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## **Phenomena, Models and Understanding**

The Lenz-Ising model and critical phenomena 1920-1971

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Phenomena, Models and Understanding  
The Lenz-Ising Model and Critical Phenomena  
1920–1971

Martin Niss

2005



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# Preface

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This dissertation has been prepared as the main component in the fulfilment of the requirements for the Ph.D. degree at the Department of Mathematics and Physics (IMFUFA) at the University of Roskilde, Denmark. The work has been carried out in the period from February 2001 to March 2005, interrupted by a leave of absence in the academic year 2002-2003 due to my reception of a scholarship to study mathematics abroad. Professor Jeppe C. Dyre was my supervisor.

## Acknowledgements

I would very much like to thank my supervisor Jeppe. From the very beginning of my dissertation work he had enough confidence in me to allow me to go my own ways. Even though he is a professor of physics proper and not a professional historian of physics, he has been keenly interested in my project throughout its duration and his door has always been open when I needed any sort of help. I would also like to thank Dr. Tinne Hoff Kjeldsen who in her capacity as a historian of mathematics has helped me greatly on numerous scholarly issues. I have also benefited very much from her help and advice on non-scholarly problems which unavoidably appear during a Ph.D. study and need to be tackled. My father Mogens Niss has provided numerous supportive comments on my project on all scales of magnitude. The linguistic appearance of the dissertation has greatly benefited from his detailed comments. Jeppe, Tinne and Mogens have all discussed the project with me during the whole period on numerous occasions, and they have read and commented on a draft of the entire dissertation. I am very grateful for their advice and commentary, but needless to say all responsibility for this dissertation solely lies with me.

At early stages of my project I discussed it with Evelyn Fox Keller, Helge Kragh, Andrea Loettgers and the Physics of Scales group at Dibner Institute comprising Babak Ashrafi, Karl Hall and Sam S. Schweber. I am grateful for all their advice. I would also like to thank Helge and Andrea as well as Anja Skaar Jacobsen and Stine Timmermann for their reading of parts of the dissertation. I am thankful for their commentary. I also wish to extend my thanks to Per Christian Hemmer and Cyril Domb, who most kindly answered some of my questions by mail at a time when the time was short and to Leo P. Kadanoff who most kindly sent me two of his books.

I also want to thank Albena Nielsen for translating Frenkel (1946) from Russian into Danish. Furthermore, I would like to thank the people of IMFUFA where my studies were undertaken. They have provided a stimulating environment and I have benefited immensely from the interdisciplinary spirit and interest in mathematical modelling which are marked features of the department.

Roskilde, March 2005

Martin Niss

### **Preface to IMFUFA Text**

This IMFUFA text is identical to the dissertation I submitted for the fulfilment of the requirements for the Ph.D. degree, except that a few minor clarifications have been made and a number of typos have been corrected.

Roskilde, August 2005

Martin Niss

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## Summary

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Modelling is an essential part of the practice of modern physicists, but this activity has not received much attention from historians of physics. The present dissertation is a step towards remedying this situation by examining modelling in one area of physics in a historical perspective, namely microscopic modelling of macroscopic phenomena in condensed matter physics from the 1920s onwards. More precisely, I focus on one single model, the Lenz-Ising model, an important model in modern condensed matter physics. However, the model is studied here because physicists' perception of the model and the role it can or should play in the understanding of macroscopic models witnessed great changes. The dissertation traces these changes in the Lenz-Ising model in its *capacity as a model*, i.e., its ability to represent physical phenomena, since its proposal in the early 1920s until the early 1970s. The dissertation focuses on this aspect of the model's history in contrast to the more technical-oriented accounts given in Brush (1967) and Hodderson, Shubert, Heims and Baym (1992) and thus presents a new side and view on the model's history.

The dissertation falls in three parts. The first part examines the roots of the model in terms of three phases with respect to the physicists' perception of the model and of the role it can play, in the epoch from 1920 to 1950. In the first phase the model was proposed by the German physicists Lenz and Ising in the early 1920s as a realistic representation of a ferromagnet. With the advent of quantum mechanics and the ensuing replacement of the foundation theory of the model, the view of the physical realism of the model changed. This in turn rendered the model irrelevant to physicists. In the third phase, which took place from the late 1930s to the 1950s, the model gained renewed interest, but now as a model of transition points in general rather than of ferromagnetism alone. The model was found to be relevant to the study of these phenomena because it could function as a proof by example that statistical mechanics can accommodate phase transitions. However, it was seen as irrelevant to a more detailed study of phase transitions because of its lack of physical realism. The driving forces behind these changes in perception of the model are analysed.

The second part of the dissertation studies how the Lenz-Ising model came to play an important role in the theory of critical phenomena of the 1960s. This was not at all in the cards in the 1950s and it is shown in the dissertation that the model was found to be physically irrelevant within three of the four areas which became the central critical phenomena in the following decade. Moreover, in these three areas more realistic models were dominant; in the field of ferromagnetism and antiferromagnetism the Heisenberg model was the preferred model, while scientists interested in the condensation of gases were preoccupied with the Mayer model. I argue that the Lenz-Ising model eventually became seen as physically relevant in the 1960s, mainly because a surprising agreement was found between the model as a representative of gases and new experimental results on argon and oxygen by Voronel' and his Russian group. This had a rub-off effect on the model as portraying magnetism.

Next, it is documented that the Lenz-Ising model toppled the Mayer model in the area of gas condensation (but not the Heisenberg model within magnetism) in the 1960s. It is argued that this was mainly due to the realisation of the mathematical difficulties involved in handling the Mayer model rather than its deficiencies as a model.

Having established that the Lenz-Ising model acquired a prominent position within the field of critical phenomena, the ways in which the model was used here are thoroughly examined. It is argued that the model was put to two different uses in the two halves of the 1960s. In the first half, the model was mainly employed to solve specific small-scale tasks, and it functioned to a large extent as a substitute for precise experimental results. It was first in the latter half of the decade that the model was put to a systematic use, namely in the fulfilment of what I term Fisher's programme. This widespread programme attempted to elucidate the correspondence between features of model Hamiltonians and critical behaviour. For this purpose, simple and tractable models were used extensively, especially the Lenz-Ising model. The latter half of the 1960s also marked the emergence of the idea that a 'universe' constituted by the Lenz-Ising model could actually tell something about real systems; an effect found in this universe, it was assumed, reveals something about the real system portrayed by the model.

This use of the Lenz-Ising model in the last half of the 1960s differs much from the previous use of models within the core areas of critical phenomena. I introduce the notion of *modelling approach* in order to describe these different modelling strategies. The notion of modelling approach is supposed to characterise different ways of using models to build phenomenological theories. The approach to modelling inherent in Fisher's programme is contrasted with two previous approaches to the 'core areas' of critical phenomena – one advanced by J. E. Mayer and one by H. N. V. Temperley.

In the final part of the dissertation, a hypothesis which I derive from a statement by Michael E. Fisher is examined, namely that the time around the late 1950s and the 1960s marks a watershed within condensed matter physics, with different approaches to modelling placed on each side of it. It is argued that this hypothesis is supported by the findings in the previous parts of the dissertation, which does indeed show such a change in the approach to critical phenomena. However, since the hypothesis concerns condensed matter physics more generally, I lay forth evidence from recollections both by protagonists of critical phenomena and by prominent solid state physicists such as P. W. Anderson, which further supports the hypothesis. However, it is beyond the scope of the dissertation to discuss the validity of the hypothesis in greater depth, so the hypothesis is laid out as a point of examination in a future research programme.

On a more general note, the dissertation argues that historical studies of the perception of models and their roles are not only worthwhile but crucial if we are to understand large parts of physics, including solid state physics or its modern counterpart, condensed matter physics. The history of the Lenz-Ising model reveals that considerable changes occurred in the perception and uses of this model. It is suggested that these changes can be explained in terms of four factors: i) the realism of the model; ii) the mathematical intricacies involved in handling the model; iii) experimental evidence; and iv) the overarching goal of modelling.

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## Dansk resumé

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Modellering er en vigtig del af moderne fysikers praksis, men denne aktivitet har ikke været genstand for meget opmærksomhed fra fysikhistorikeres side. Herværende afhandling tager et skridt hen mod at afhjælpe denne situation ved at undersøge modellering i et område af fysikken i et historisk perspektiv, nemlig mikroskopisk modellering af makroskopiske fænomener fra 1920'erne og fremefter. Mere præcist fokuserer jeg på en enkelt model, Lenz-Ising-modellen, som er en vigtig model i moderne faststoffysik. Modellen studeres imidlertid her fordi fysikernes opfattelse af modellen og de roller den kan spille har undergået store forandringer. Afhandlingen afdækker disse ændringer i modellens *modelkapacitet*, dvs. dens evne til at repræsentere fysiske fænomener, i tiden fra den blev foreslået i 1920 frem til starten af 1970'erne. Afhandlingen fokuserer på dette aspekt af modellens historie i modsætning til mere teknisk-orienterede behandlinger givet i Brush (1967) og Hoddeson, Shubert, Heims and Baym (1992) og præsenterer herved både en ny side af og et nyt blik på modellens historie.

Afhandlingen består af tre dele. Den første del undersøger modellens rødder ud fra tre faser med hensyn til fysikernes opfattelse af modellen og den rolle modellen kan spille i perioden 1920 til 1950. I den første fase blev modellen foreslået af to tyske fysikere Lenz og Ising i de tidlige 1920'ere som en realistisk repræsentation af en ferromagnet. Med fremkomsten af kvantemekanikken og den efterfølgende udskiftning af modellens grundlæggende teori, ændrede fysikernes syn på modellens realisme sig. Den tredje fase fandt sted fra sidst i trediverne til 1950'erne. Her var der fornyet interesse for modellen, men nu som en model for overgangspunkter generelt fremfor ferromagnetisme alene. Modellen blev opfattet som relevant for studiet af disse fænomener fordi den gav et eksistensbevis for at statistisk mekanik kan udvise faseovergange. Den blev imidlertid set som irrelevant for en nærmere undersøgelse af virkelige systemer pga. mangel på fysisk realisme.

Anden del af afhandlingen studerer hvordan Lenz-Ising modellen kom til at spille en vigtig rolle i teorien for kritiske fænomener i 1960'erne. Dette lå overhovedet ikke i kortene i 1950'erne og afhandlingen dokumenterer at modellen blev opfattet som fysisk irrelevant indenfor tre ud af de fire områder som blev opfattet som centrale kritiske fænomener i det efterfølgende årti. Dertil kommer at mere realistiske modeller var dominerende indenfor disse tre områder i 1950'erne; indenfor ferro- og antiferromagnetisme var Heisenberg-modellen den foretrukne, mens fysikere interesserede i kondensation af gasser var optagede af Mayer-modellen. Jeg argumenterer for at Lenz-Ising-modellen blev set som fysisk relevant i 1960'erne hovedsageligt fordi man opdagede en overraskende overensstemmelse mellem modellen som en repræsentation af gasser og nye eksperimentelle resultater for argon og ilt af Voronel' og hans russiske gruppe. Dette havde en afsmittende virkning på modellen som afbildende magnetisme.

Dernæst dokumenteres det at Lenz-Ising-modellen overvandt Mayer-modellen indenfor gas kondensation (men ikke Heisenberg-modellen indenfor magnetisme) i 1960'erne.



Der bliver argumenteret for at dette hovedsageligt ikke skyldtes Mayer-modellens mangler som model, men at man indså at de matematiske problemer involveret i undersøgelsen af Mayer-modellen var for store.

Efter at det således er etableret at modellen fik en fremtrædende position indenfor kritiske fænomener, undersøges måderne som modellen blev brugt til at opnå indsigt grundigt. Der argumenteres for at modellen blev brugt forskelligt i de to halvdele af 1960erne. I den første halvdel blev modellen hovedsageligt anvendt til at løse små specifikke opgaver og den fungerede i vid udstrækning som en erstatning for præcise eksperimentelle resultater. Det var først i den sidste halvdel af årtiet at modellen blev brugt mere systematisk til at udfylde hvad jeg har kaldt Fisher's program. Dette vidt udbredte program forsøgte at belyse sammenhængen mellem træk ved Hamilton-operatorer for modeller og kritisk opførsel. Til den ende blev simple og undersøgelsesbare modeller brugt i stor stil, især Lenz-Ising-modellen. Den sidste halvdel af 1960erne markerede også fremkomsten af den ide at det univers som Lenz-Ising-modellen skaber rent faktisk kan sige noget om virkelige systemer – en effekt som findes i universet siger noget om virkelige systemer.

Denne brug af Lenz-Ising-modellen i 1960erne afviger meget fra tidligere tiders brug af modellen indenfor dele af kritiske fænomener. Jeg introducerer begrebet modelleringstilgang for at karakterisere forskellige måder at bruge modeller til at bygge fænomnologiske teorier. Modelleringstilgangen i forbindelse med Fishers program kontraheres med to tidligere tilgange indenfor kritiske fænomeners 'kerneområder' – én fremsat af J. E. Mayer og én af H. N. V. Temperley.

I den sidste del af afhandlingen undersøges en hypotese jeg afleder af en påstand som Michael E. Fisher er fremkommet med. Hypotesen siger at tiden omkring 1950erne og 1960erne markerer et skel indenfor faststoffysik med to forskellige modelleringstilgange på hver side. Der argumenteres for at denne hypotese understøttes af afhandlingens tidligere resultater som viser en sådan ændring i tilgangen til kritiske fænomener. Fordi hypotesen angår faststoffysik mere generelt end blot kritiske fænomener, fremlægger jeg dokumentation i form af erindringer af hovedpersoner indenfor både kritiske fænomener og faststoffysik, såsom P. W. Anderson, som yderligere støtter hypotesen. Det er imidlertid udenfor afhandlingens rækkevidde af diskutere hypotesen mere grundigt, så dette lægges ud som et fremtidigt forskningsprogram.

Overordnet set mener jeg at afhandlingen viser at historiske studier af opfattelsen af modeller og deres rolle ikke alene er værdifulde, men er væsentlige hvis vi vil forstå en stor del af moderne fysik, nemlig faststoffysik. Lenz-Ising-modellens historie afslører at der sker store ændringer i opfattelsen af denne model og hvordan den bruges. I afhandlingen argumenterer jeg for at disse ændringer kan blive forklaret ud fra fire faktorer: i) modellens realisme; ii) matematiske problemer involveret i undersøgelsen af modellen; iii) eksperimentel evidens; og iv) det overordnede formål med modellering.

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During the last years of my studies at Roskilde University for a master's degree in physics and mathematics, I encountered Rodney Baxter's book on exactly solved models in statistical mechanics.<sup>1</sup> I was quite surprised to see that he advanced the view that the Lenz-Ising model (or the Ising model as most physicists call it<sup>2</sup>) plays an important role in the modern theory of so-called critical phenomena (critical phenomena are a special type of phase transition; see chapter 2). Ever since my encounter with this model at a course in statistical mechanics, I had thought that it was merely of pedagogical value, because how could such an extremely simple and unrealistic model say anything about real systems? In fact, I felt like one of the 'down-to-earth' physicists and chemists, Baxter described in his preface, "[...] who reject lattice models as being unrealistic. In its most extreme form, their argument is that if a model can be solved exactly, then it must be pathological."<sup>3</sup> Not only did Baxter accept a type of models (lattice models) which, according to himself, some scientists reject, his underlying modelling strategy was quite radical. At the department where I did my studies, technical and philosophical analysis of modelling in science receives a lot of attention. The modelling strategy advocated by Baxter seemed to be at variance with at least some of the strategies I had encountered during my studies. One widespread strategy is to start with one reasonable model and then get a series of successively refined models, but Baxter seemed to advocate the view that one should employ a host of extremely simple models – the one more unrealistic than the other.

My encounter with Baxter's monograph made me think about the role of statistical mechanical models in modern physics: It seems like there are different views as to which models are acceptable and which are not and my own experiences suggested divergent strategies for obtaining knowledge based on models. Is it correct that there are such different views and strategies? Moreover, are they subject to change over time? After I had graduated and chosen to pursue a career in the history of physics rather than physics proper, I found it natural to follow these ideas and study the role of statistical mechanical models from a historical perspective. From such vague ideas grew the present dissertation.

On a more scholarly note, I believe that such a study is not only worthwhile but crucial for understanding the actual practice of physicists. Most physicists would agree that the invention, manipulation, experimental comparison and adjustment of models are crucial parts of doing physics. In fact, several physicists would say that the handling of models is the way they get hold of the world. A model differs from both experiments and the theories applied in the building of the model and it occupies a different place within science.<sup>4</sup> For instance, I agree with the philosopher Margaret Morrison's idea that models

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<sup>1</sup>See Baxter (1982).

<sup>2</sup>Since the role played by Wilhelm Lenz is on par with the one of Ernst Ising, I shall follow Brush (1967) in naming the model after both physicists.

<sup>3</sup>(Baxter; 1982, p. v).

<sup>4</sup>I have much sympathy for the philosophical programme behind 'the models as mediators group'(Morgan

are autonomous agents. In addition to their autonomous status, models have a unique feature which is of special importance: By its very definition – I define a model as a simplified representation of a section of reality – a model does not give a faithful picture of a situation or phenomenon. So, models occupy a prominent place in physics and they are autonomous in relation to theories and experiments.

Despite the prominent position of models in physics, no systematic historical account of questions such as the above about the perception and roles of models has been produced yet. As a matter of fact, most aspects pertaining to models in their capacity of being *models*, i.e., simplified representations, have not received the attention they deserve from historians of science<sup>5</sup> (in recent years models have attracted the interest of philosophers of science). Consequently, I think that modelling in the sciences should be taken up in earnest by historians of science and I want to strike a blow for considering models and modelling from a historical perspective.

By way of an example of the importance of such inquiries, a quotation by Michael E. Fisher, a distinguished condensed matter physicist,<sup>6</sup> about his discipline, will do. According to Fisher a shift occurred in condensed matter physics around the 1950s and 1960s:

So the crucial change of emphasis of the last 20 or 30 years that distinguishes the new era from the old one is that when we look at the theory of condensed matter nowadays we inevitably talk about a ‘model’. (Fisher; 1983, p. 47)

Fisher says two things. First, models have acquired great importance in condensed matter physics; now novel phenomena in this area are approached with models rather than the comprehensive and systematic theories used previously. More significantly for the purpose here, he talks about two eras of condensed matter physics. From the context of his writing it is clear that he refers to two fundamentally different ways of using models in what he calls the task of the theorist – i.e., how the theoretical physicist looks at the real world and tries to understand it. I shall return to Fisher’s quotation shortly; the important point here is that Fisher thinks a considerable change happened in the way the theoretical physicist works as a result of a change in the modelling practice. This example suggests that if we wish to describe and understand changes in the practice of the physicist within a huge area of physics, such as condensed matter physics, we need to focus on his or her use of models in the pursuit of knowledge. This is my overarching point, which will be illustrated for the specific case of critical phenomena.

## 1.1 The Central Questions of the Thesis

There are numerous issues covering the handling of models and the use of models to obtain knowledge that deserve to be considered. This dissertation concentrate on physicists’

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and Morrison; 1999) which argues that models are mediating between theory (in the sense of foundational theory) and experiments.

<sup>5</sup>One notable exception is a paper by Schweber and Wächter (2000). It discusses the relation between models (in condensed matter physics and quantum chemistry) and the foundational theory used in the modelling process.

<sup>6</sup>Condensed matter physics is the umbrella term used since the 1960s for what was previously known as solid state physics and the theory of liquids.

perception of the ability of models to represent particular phenomena. What factors determine whether a model is perceived as capable of modelling a situation or not?<sup>7</sup> Are these factors subject to change over time? Given that several different models are found capable of representing a given phenomenon, what criteria determines the choice of one of them over the others? Do these criteria change with time?

It is not only the perception of a particular model which changes; the above quotation by Fisher illustrates that also the way models are conceived and put to use in condensed matter physics more generally may be changing. However, except for the shift of focus from theory to model, he did not elaborate on the precise content of this change and he did not provide a historical account. Therefore, I will take his statement as a *hypothesis* in need of testing rather than as a solid fact.

So, the reader will find two overarching themes in this dissertation. The first theme concerns the development in the perception of a particular model and how a specific phenomenon should be modelled. The second theme is an examination of the hypothesis: is it possible to discern two eras characterised by two different perceptions of models? Concerning the latter question, since it is beyond the scope of the dissertation to test the hypothesis for all of condensed matter physics attention will mainly be restricted to one area, that of critical phenomena. The findings concerning this area will be used in an attempt to shed light on condensed matter physics in general, without attempting to provide a more general, systematic discussion of this question.

These two themes are quite general and wide-ranging, so I have taken the development of a single model as my point of departure. The Lenz-Ising model is a good case for both a discussion of changes in the perception of one particular model and possible driving forces behind such changes, and as a starting point for testing the hypothesis of a fundamental change in condensed matter physics at large. From a modern point of view, the Lenz-Ising model can represent several different physical (and some non-physical!) phenomena in the real world. However, every physicist agrees that almost irrespectively of the physical system in question, the Lenz-Ising model simplifies greatly the features of the system. Thus it is not only clearly a model, but one where its characteristics as a model are of central importance. When it comes to its status within physics, the model is cited in most textbooks on statistical mechanics and in a large number of books on condensed matter physics. In addition, with more than 2500 papers published about it since 1945,<sup>8</sup> its place as an essential contribution to physics is secured. That the model is not just a marginal ‘pathological’ case is revealed by the fact that it can be viewed as a characteristic example of a certain class of physical models, simple statistical-mechanical models, which also include models such as the Heisenberg model, the Potts model, and the spherical model.

More importantly, the historical development of this model shows that the perception of it changed dramatically. It was originally proposed as a good representation of ferromagnetism,<sup>9</sup> but this changed within the first decade of its ‘life’ and since the 1940s and 1950s, it had the status of being irrelevant within this field. However, in the 1960s the model acquired an advanced position within the field of phase transitions and critical phenomena. This view is expressed, for instance, in the textbook by Binney et al. (1992):

<sup>7</sup>The question whether or not a particular model is capable of representing a situation typically cannot be answered by ‘yes’ or ‘no’, but involves compound answers like ‘on the one hand . . . , but on the other . . . .’ This makes the situation more messy, but I still believe it is possible to examine this question.

<sup>8</sup>According to a run performed in 2004 on Science Citation Index for the number of papers citing either Ising (1925) or Onsager (1944).

<sup>9</sup>A ferromagnet has a magnetisation even in zero external field (if the temperature is low enough).

“Far and away the most influential model of a system capable of a phase transition is the *Ising model*.”<sup>10</sup> Furthermore, it will be argued that the crystallisation of the view that the Lenz-Ising model is actually capable of representing these physical phenomena caused a change in the epistemological perception of modelling in this field more generally, so that a new approach to modelling appeared.

Out of the above considerations grew five questions that directed my studies of the history of the Lenz-Ising model from its proposal in the early 1920s to the late 1960s.

The Lenz-Ising model appeared shortly before the advent of the new quantum mechanics, and it was based on the old quantum theory. The *first question* concerns the impact of this change of the foundational theory on the perception of the model:

*What role did the new quantum mechanics have for the perception of the Lenz-Ising model in its capacity as a model? And, how did this model ‘survive’ the change of fundamental theory?*

Due to the coincidence of the appearances of the Lenz-Ising model and quantum mechanics, the process of answering this question also establishes the origins of the Lenz-Ising model.

The *second question* is why it became, if not the only model, then the preferred model within the field of critical phenomena in the 1960s. Since the 1930s, several physicists perceived it as interesting because they conjectured that it possesses two important abilities: exhibition of a phase transition and mathematical tractability. A possible display of a phase transition was deemed important as a proof by example that equilibrium statistical mechanics is able to deal with such transitions. However, the model was not thought to yield more direct insight into phase transitions in general and critical phenomena in particular. This attitude was shared by most physicists of the 1950s, but in the 1960s a new attitude emerged. So, the question is:

*Why was it realized in the 1960s that the Lenz-Ising model could contribute in an essential way to the understanding of critical phenomena?*

Moreover, the model acquired a prominent place at the expense of another model which had previously been studied in the field of critical phenomena of the liquid-gas transition. The *third question* concerns this point:

*Why did the Lenz-Ising model topple the other model?*

Returning to the second question, the answer to it established the reasons for the change in the perception of the Lenz-Ising model from irrelevance to relevance for the study of physical phenomena, it is natural to ask what consequences this had for the perception of the role of models within the field of critical phenomena. So the *fourth question* is:

*Did the perception of the role of models within the field of critical phenomena change fundamentally or was it unaffected by the realisation of the relevance of the Lenz-Ising model?*

More specifically, it is examined whether a change occurred in two respects. The first respect concerns which models were acceptable and which were not, while the second respect is of an epistemological nature: how do models give us insight into real systems?

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<sup>10</sup>Binney et al. (1992), p. 55; emphasis in the original.

If such a change occurred, it may well be what Fisher had in mind in the above quotation and it is used as a starting point for a discussion of the hypothesis derived from his statement: What do the changes established previously have to say about the hypothesis? The *fifth question* concerns this hypothesis more generally:

*Is the hypothesis of two distinct eras in condensed matter physics correct?*

## 1.2 Demarcations

One restriction in the examination have already been mentioned, namely to models in condensed matter physics. The extent to which the conclusions of the dissertations are related to other areas of physics will not be discussed in depth.

The goal is to determine factors involved in the perceptions of models and changes in these perceptions. The most significant restriction imposed is to focus mainly on *scientific* factors. This should not be taken as a dismissal on my part of the importance of ‘external’ factors for scientific development. In fact, I do acknowledge that factors of an extra-scientific nature could well be involved on two levels. On one level, the contingent aspect of modelling, i.e. that models are not simply derived from theory, gives room for physicists’ personal choices and tastes in the determination of which models are acceptable and which are not. For instance, it is very likely that a scientist’s training influences, in subtle ways, his or her approach to modelling. However, scientific factors, such as the relation between a model and foundational theory, the role of experiments, etc., obviously do have an important impact on the perception of models and changes therein. Therefore, it makes sense to restrict the attention in this study to such factors, and to postpone a study of the influence of cultural and social factors to future studies.

On another level, extra-scientific factors may very well influence the *changes* in the perceptions of models and modelling over time. What I want to do with respect to these changes is *not* to explain them, but rather to *describe* their scientific content. An explanation would demand that extra-scientific factors to be taken into account, but for this study these are not necessary.

The questions posed in the previous section have been used to define the degree of detail in the treatment of the development of the Lenz-Ising model. This means that aspects of this development have only received the attention needed to answer these questions – that is, what can be termed the ‘core of the matter razor’ have been applied. It is worthwhile to touch briefly upon some of the restrictions made in this respect.

First, the technical mathematical aspects of the matter will not be examined to any appreciable degree. For instance, I shall neither look into what mathematics was applied to solve the three-dimensional Lenz-Ising model, nor consider where the person who solved this model acquired the necessary skills to perform his mathematical analysis. The interested reader can find much information on this issue in Krieger (1996). On the other hand it is obviously important to establish that the mathematical difficulties involved in manipulating the models did in fact have an impact of how physical phenomena were modelled. In short, mathematical methods are only examined to the extent that they were judged to be important for the perception of the ability of the models to represent physical phenomena.

The core of the matter razor has also been applied to experiments, with a similarly minimalistic result: Experimental results are treated in so far as they are judged to have influenced the perception of models in this field and in sufficient detail so as to allow for



an understanding of this influence, but it is beyond the scope of the dissertation to treat them in any more detail. For instance, even though I think it is interesting to map the developments that led to a host of experiments precise enough to test the predictions of the simple models in the 1960s, this has been left out in my pursuit of conclusion.

Some might look for a coverage of computer simulations and the renormalisation group technique – this will be in vain. The use of Monte Carlo simulations of models did indeed start in the period under study. According to Brush (1964) F. J. Murray proposed a Monte Carlo method for the Lenz-Ising model already in 1952. The general view of the period seems to be that this method was too inaccurate to be useful, even though there was some controversy about its accuracy.<sup>11</sup> Consequently, Monte Carlo simulations have not been taken into account.

Concerning the renormalisation group technique,<sup>12</sup> it will be documented that the intensive interest in the Lenz-Ising model was initiated in the 1960s (the curve of the number of references to Ising (1925) or Onsager (1944), the two most important references to the Lenz-Ising model, of Appendix A, supports this assertion). Moreover, it will be argued that the ideas about what role the Lenz-Ising model should play were advanced in the same decade. This means that the important ideas about modelling appeared prior to the advent of the renormalisation group technique of the 1970s. Even though I acknowledge that this important technique had a large impact on the justification and reception of the new ideas about modelling, I think it is legitimate to omit this otherwise important development in my account of how it was realised that the Lenz-Ising model is capable of describing the phenomena in question. Of course, the justification and reception of the new approach is an interesting question (yet beyond the scope of the present dissertation), but I think it is both possible and reasonable to neglect the renormalisation group technique in the present endeavour.

### 1.3 Methodological Reflections

It is necessary briefly to reflect upon how the perception of a particular model is to be uncovered from the sources available, because this question is not usually treated in historical work. The main purpose is to chart the attitude shared by physicists towards the Lenz-Ising model over time. In order to be able to say something about divergent attitudes, the perceptions of selected scientists need to be determined. The ways to fulfil these two demands have something in common, but they do also differ and raise questions of their own.

<sup>11</sup>See Sykes and Fisher (1962), pp. 920–921 and Domb (1996), p. 359.

<sup>12</sup>To quote The Panel on Condensed-Matter, National Research Council about the renormalisation group methods:

These techniques are useful in dealing with physical phenomena in which there exist fluctuations that occur simultaneously over a wide range of different length, energy, or time scales. The method proceeds by stages, in which one successively discards the shortest-wavelength fluctuations until a few macroscopic degrees of freedom remain. The effects of the short-wavelength fluctuations are taken into account approximately at each stage by a *renormalization*, i.e., change in magnitude, of the interactions among the remaining long-wavelength modes. [...] Their use has provided a theoretical understanding of empirical relations among different properties near the phase transition or critical point of a given system and has made it possible to predict critical properties with a high degree of accuracy. (Panel on Condensed Matter Physics; 1986, p. 11)

I shall start with some reflections about how to get hold of the attitude of a particular scientist. Since the role(s) of models in the actual practice of physicists and what counts as valid arguments for and against models are the focal points, their handling of models become of central importance, that is how they use models in concrete situations to obtain insight into a particular phenomenon.

There are five types of contemporary, published material which can be used to extract information about a given physicist's perception of the model. First of all there are the original research papers, which come in three variants with respect to models. The first variant is, of course, the one where a new model is introduced. Here important parts of the perception of the models in their capacity as models will typically be discussed, including matters such as the status of the model, the task it is supposed to perform, either in the paper or in the long run if the model is intractable for the author. The second variant is the presentation of a new mathematical result about the model. The author will more often than not either repeat the received view of the model or militate against it, and again this gives valuable information. The last of the three types of original research papers concerns the application of the model, often to interpret an experiment, but sometimes to the study of another, physically more relevant model. It should be noted that a single research paper can combine several of these three types of research papers. The last two of the five types of published sources are review papers and survey type monographs, on the one hand, and textbooks, on the other. The longer format of the two former types implies that they are often quite explicit in their statements about the role of a model, its status, the degree of confidence one should have in it, etc. This applies even more to the textbooks which have the further advantage of representing a more consolidated form of consensus knowledge at the time of publication.

A scientific paper cannot be used uncritically as a source of detailed information about the author's view; the published manuscript is the product of a review and revision process where editors and referees have participated in the shaping of the final version of the manuscript.<sup>13</sup> So, when I ask about the view of a particular scientist, I do not rely on published material alone, but have resorted to other sources as well, for instance Ph.D. theses, correspondence, interviews, and autobiographical material. Of course, these sources present problems of their own which have to be taken into account, but it is possible to form an adequate picture of the scientist's view from a combination of them.

A related problem is what happens if the scientist does not publish anything about the model at all – we may still be interested in his or her view, for instance, because he or she advocated a rival model. how do we determine this view in that case? When I embarked on this project, I thought that unpublished material accessible in archives would provide valuable sources for physicists' arguments of the deficiencies and merits of models and more general discussion of the role of models, so that the views of scientists who have not published on a given model could be derived from this material. Unfortunately, the archives I have consulted<sup>14</sup> contained disappointingly few remarks of this kind. In the few cases where I want to identify the view of a particular scientist who has not published anything about the model, other sources must be taken into account, for instance biographical material.

Turning to the entire community dealing with, say critical phenomena, it is relevant to establish two issues: first, whether there is a common attitude within the community

<sup>13</sup>See, e. g., Kragh (1987).

<sup>14</sup>The Onsager Archive in Trondheim, Norway, the Joseph E. Mayer archive in San Diego, The Peierls Archive in Oxford, the Kramers Archive at the Niels Bohr Archive.

towards a particular model and second, if this is the case, how this attitude develops over time. This gives rise to the problem of how to determine the attitude within such a group at a given time? Of course one can consult textbooks of the past, which will often provide a consensus view on an issue. Unfortunately, the number of relevant textbooks in the period under study is not very large, so it is often necessary to epitomise the views expressed in the research papers of the group. In this situation the above problem with the review and revision process is not relevant because here there is no need to discern the view of a single scientist from the view of the editor/referee. The paper in question expresses something in between their views, which is the relevant one to this issue. However, in some situations the number of papers about a particular model is low (this is the situation for the Lenz-Ising model in the middle of the 1950s), so only a few original research sources are available for an assessment of the perception of the model. In such situation, I have involved other sources as well, mainly recollections by scientists, but one of the rare textbooks.

The over 2500 articles published on the Lenz-Ising model are a blessing because they constitute a comprehensive material, but they are also a curse since it is obviously too large a task to go through all of them. Even though the number of papers for the period until the 1970s is smaller, the problem is the same. In order to remedy it, I have to a large extent followed the advice of Söderqvist (1997) and relied on Science Citation Index in my search for the pivotal papers of the period.

## 1.4 Contributions to History of Physics

In this dissertation, I document the changes in the perception of a particular model, the Lenz-Ising model, from being deemed irrelevant to obtaining an important place within the field of critical phenomena. Even though the prominent position of the model in modern physics alone merits an examining of its history, the contribution to the history of physics goes beyond the history of this particular model.

This study of changes contributes to a quite general research programme which I propose, namely that of examining and explaining changes in the perception of modelling in physics. It is asserted above that modelling is an important aspect of the practice of physicists, so it is important to understand changes in the perception of modelling. On a general level, the study of the Lenz-Ising model provides an existence proof that drastic changes do occur in the perceptions of a model and thus points out the relevance of such studies of the development in the perception of models.

Less generally, the studies presented here contributes to this research programme in three respects. First, I point out that the development of the perception of the Lenz-Ising model in the period 1920 to circa 1970 can be described as an interplay of four factors: the realism of the model, solutions to mathematical problems arising in dealing with the model, agreement with experimental results and epistemological perceptions of how models contribute to the understanding of physical phenomena. It will be argued that these four factors are sufficient for a description of the development in the perception of the model.

The second respect the studies contribute to the research programme is through my introduction of the notion of *modelling approach*, which tries to capture the essential, overarching features of an approach to modelling taken by a scientist or a group of scientists. Modelling approach is supposed to describe the features of physicists' general dealing with

models in their pursuit of insight into physical phenomena. The modelling approach will be employed to describe the specific transition from one approach to modelling of the 1950s to a new one of the 1960s. However, I believe this notion can be applied, perhaps after some modifications, to other epochs and fields of physics.

The third and final respect in which the studies contribute to the general programme is by discussing the hypothesis based on Fisher's assertion described above, i.e. the extent to which the changes charted in the first parts of the dissertation is part of a greater movement within condensed matter physics. This examination, while necessarily of a less well-documented nature, points out fields where this hypothesis could be tested.

To my knowledge this is the first systematic study of the driving forces behind changes in the perception of individual physical models and the effect of such changes on the attitudes towards the purposes of modelling.

## 1.5 Taking Stock of Secondary Sources

The views of many of the protagonists in the development of a theory of critical phenomena in the 1960s and 1970s are beginning to be documented. Quite a few of them have recounted various aspects of the history.<sup>15</sup> Moreover, several of the protagonists have published recollections of varying lengths, either of their own contributions<sup>16</sup> or those of other scientists.<sup>17</sup> Cyril Domb is the one who has written most extensively on the history of critical phenomena in several papers<sup>18</sup> and a lengthy monograph.<sup>19</sup> The monograph is especially important because it recounts the history of the technical side of the investigation of the Lenz-Ising model from Onsager and onwards. While I have some reservations about aspects of Domb's account, I find his description of the technical development sober.<sup>20</sup>

Turning to the works of historians of physics, Stephen G. Brush has written on the history of critical phenomena in general and the Lenz-Ising model in particular. Brush (1983) contains a fairly brief account of the development of the theory of phase transitions, while Brush (1967) concentrates on the history of the Lenz-Ising model. Both are valuable sources about the technical development of the various theories and models in question, but neither deals thoroughly with the model in its capacity as a model. The same applies to a chapter by L. Hoddeson, H. Schubert, S. J. Heims and G. Baym on collective phenomena (to which the Lenz-Ising model belong) published in a pioneering book on the history of solid state physics.<sup>21</sup> 'The Physics of Scales' project conducted by the collective of Babak Ashrafi, Karl Hall and Sam Schweber,<sup>22</sup> has made a host of valuable material on the history under study available at the internet,<sup>23</sup> even though the focus of this project

<sup>15</sup>For instance, Allan Franklin arranged a symposium on the history of critical phenomena at the March APS Meeting in Los Angeles, 20 March 1998. Here the actors Johanna M. H. Levelt Sengers, Mikhail Anisimov, Michael E. Fisher, P. C. Hohenberg and Valery L. Pokrovsky, presented papers on the history of critical phenomena. Abstracts were published in *History of Physics Newsletter* Volume VII, No. 3, August 1998.

<sup>16</sup>Domb (1990), Yang (1995), and Yang (1983).

<sup>17</sup>Fisher (1996) and Domb (1991) have written about each other.

<sup>18</sup>Domb (1971), Domb (1985), and Domb (1995).

<sup>19</sup>Domb (1996).

<sup>20</sup>I haven't checked the book systematically, but to the extent that I have read the primary sources, I think it gives a correct description of what concretely happened, even though he tends to neglect his own contribution.

<sup>21</sup>Hoddeson, Shubert, Heims and Baym (1992).

<sup>22</sup>This project is part of the 'History of Recent Science and Technology' project hosted at the Dibner Institute, MIT.

<sup>23</sup>At the website <http://hrst.mit.edu/hrs/renormalization/public/>

differs from mine. Two parts of this work of considerable relevance to the present project deserves mention, namely that of providing a time line for the development and the publication of numerous interviews with the protagonists in the field.

However, none of these sources systematically discussed the development in the perceptions of models within the area of critical phenomena, which is the subject in the present dissertation. There are some scattered remarks on this matter, but no detailed account is given. On the other hand, this material provides an excellent background for the present study. In fact, the task I have set out to accomplish would have been much larger if, for instance, Domb's book had not been available.

Turning to the philosophical literature on models in science, it is enormous both in terms of quantity and in the issues addressed. One could have hoped that this literature would provide notions relevant for an analysis of historical studies and case studies of particular models. None of it, however, seems to provide a framework for a discussion of different approaches to modelling.

The philosophical literature on models in general is, for obvious reasons, preoccupied with philosophical problems, such as the general relation between model, theory, and experiment. I have found these discussions too general and broad to provide much inspiration for the issues of this dissertation, which pertain to different approaches for obtaining insight into specific physical phenomena from models based on the same foundational theory. In fact, I have only found inspiration in the work of Stephan Hartmann, whose notion of story will be discussed later in this dissertation.

As regards the more specific literature on statistical mechanical models, it does in fact discuss phase transitions and critical phenomena in general and the Lenz-Ising model in particular. However, in most of the literature<sup>24</sup> both the Lenz-Ising model and critical phenomena are used as case fuel for general philosophical discussions, for instance to criticise philosophical theories of approximation and idealisation, rather than being used to address questions pertaining to different strategies for obtaining insight into physical phenomena. There is one exception, though: The philosopher Robert W. Batterman delivers a philosophical defence for the use of what he calls minimal models (which are called caricature models here) instead of more realistic models.<sup>25</sup> What is done in this dissertation is essentially to examine how physicists came to the same result as Batterman. Unfortunately for the discussion here, his arguments are not similar to the ones used in the historical development under study here, so his account does not shed much light on the arguments which were actually put forward historically.

## 1.6 Organisation of the Dissertation

The bulk of the dissertation falls in three parts, but before those comes a *prologue*. This chapter sets the stage for the rest of the dissertation. I have extracted some general principles of modelling in solid state physics which were shared by all the scientists considered in this dissertation from the 1920s and onwards. Moreover, the chapter contains some important terminology.

The *first part* of the main matter deals with the first question of section 1.1 and covers the years 1920 to circa 1950 in the history of the Lenz-Ising model. In other words, this part discusses the birth of the Lenz-Ising model, its negative reception after the advent of

<sup>24</sup>This applies to Hughes (1999), Liu (1999), Liu (2004).

<sup>25</sup>Batterman (2002).

the new quantum mechanics, and why the model did not fall into oblivion even though it was dismissed as a model of ferromagnetism. This part of the history has been treated by others, mainly Brush (1967) and Hoddson, Shubert, Heims and Baym (1992), but they focused on the development in the *mathematical* examinations of the model rather than the modelling aspect as such. The main point of this part is to establish this side of the history, but it also critically examines some of the conclusions of the earlier expositions based on new material, which leads to revisions of these conclusions.

This part consists in a reproduction of my paper – published in *Archive for History of Exact Science* – which reports research done during my doctoral studies.<sup>26</sup>

*Part Two* examines the second, third and fourth question of section 1.1. Chapter 7 documents that the model as a representation of the core areas of critical phenomena was, by and large, perceived as physically irrelevant in the 1950s. The next chapter deals with the second question of section 1.1, viz. why it was realised that the Lenz-Ising model could contribute to the understanding of critical phenomena. This is followed up by a discussion of the third question – why the so-called Mayer model was toppled by the Lenz-Ising model – in Chapter 9. Having established that the Lenz-Ising model can in fact contribute to the understanding of critical phenomena, Chapters 10 and 11 examine how the model was used more specifically to gain this understanding in the two halves of the 1960s. Chapter 12 discusses the change from the 1950s to the 1960s in how these phenomena are modelled in terms of the notion of modelling approach.

The fifth question of section 1.1 is discussed in *Part Three*. As noted above, a thorough examination of the hypothesis involved in this question is way beyond the scope of the present dissertation. Instead, it is examined what the two previous parts have to say about the hypothesis, but I also give a sort of survey of some material from other areas that I have encountered during my studies which shed light on the hypothesis. However, I would like to stress that this survey is not meant as neither a systematic nor a comprehensive account of the issue. Rather it outlines a programme for future research.

A graph of the number of papers in Science Citation Index citing either Ising (1925) and/or Onsager (1944) can be found in Appendix A. Even though not every paper on the Lenz-Ising model cites one or both of these two sources, especially in the last two decades, this graph gives a rough impression of the development in the number of papers on this model. Furthermore, Appendix B is a compendium of the various guises of the Lenz-Ising model.

Finally, I should say that in the dissertation, I have used the convention that text in square brackets [] is my remarks, unless otherwise stated.

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<sup>26</sup>See Niss (2005a).



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## Prologue

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This chapter provides a framework for the remainder of the dissertation. Its main purpose is to clarify some conceptual and terminological points of importance to what follows. First, the notion of model used throughout the dissertation is presented and discussed. Next, the chapter describes the common features of modelling in the parts of physics and the epoch considered.<sup>1</sup> Then two important notions, *the perception of a model* and *the role of a model*, are characterised by means of general terminology about modelling. Finally, another pair of terms, explanation and understanding, are briefly introduced.

### 2.1 The Notions of Model and Theory

The concept of model is a very diffuse one, laden with different connotations to different people. I have above defined a model as a simplified representation of a section of reality. Even though this definition is not likely to satisfy everyone's intuition of a model – for instance it excludes the standard use of the notion in model theory in mathematics – I believe it captures the essence of the physicists' notion of model.<sup>2</sup> So, by definition a model is a representation of some real system, but the very concept of model implies that the model is based on some kind of simplifying particular assumptions which are not simply derived from a foundational theory. Since it is rarely obvious what are the significant features of the phenomenon represented by a given model and what are the insignificant ones, a choice has to be made. The fact that models are not simply derived from theory implies that the modelling process involves a large element of freedom to choose which additional assumptions to base the model on.

There is no sharp distinction between what is called a model and what is called a theory in physics, since most theories also involve some kind of simplification. However, the physicists dealt with in this dissertation do in fact distinguish between 'theory' and 'model.'<sup>3</sup> To them, a model is a representation of a specific physical phenomenon, while a theory applies to a large range of phenomena in contrast to the smaller radius of application of a model. I think they would subscribe to the definition of a theory, on the other hand, as "A general, systematic account of a subject matter."<sup>4</sup>

One should distinguish between two types of theory: foundational theory and, in lack of a better term, phenomenological theory. The foundational theory (some would say 'effective field theory'<sup>5</sup>) – in most cases dealt with here this is quantum mechanics – gov-

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<sup>1</sup>I believe that my description goes beyond the field considered in this dissertation and applies to a large part of what a later time called condensed matter physics.

<sup>2</sup>A good concise description of philosophical issues of scientific models is given by Frigg and Hartmann (2005).

<sup>3</sup>There are a few exceptions to this rule, but they will be mentioned explicitly.

<sup>4</sup>Taken from the entry "Theory" in Boyd et al. (1992).

<sup>5</sup>See Schweber and Wächter (2000).



erns the behaviour of the constituents of the model. A phenomenological theory could for instance be a theory of critical phenomena.

Sometimes a phenomenological theory is based on a few, fundamental principles, but it need not be so. What was termed the theory of critical phenomena in the 1960s was not based on such principles. Rather the theory consisted in a conglomerate of components: exact results about statistical mechanical models, rigorous proof about the behaviour of classes of models, rigorous thermodynamical arguments placing constraints on the models, analogy considerations, partly unjustified hypotheses etc. The character of this theory of critical phenomena was not monolithic. I think the term ‘theory’ used here can be described as a network of concepts, models and results derived from a fundamental theory. This network was hierarchical, so it was clear how each of the above components fitted together and issues of priority could be settled. Moreover, the theory was required to be coherent and consistent.

In some cases a single model will qualify as a theory, but there seems to be a requirement that the model then has to be theoretically well-grounded. One possibility is that the model, while a simplified representation of the situation under study, is perceived as a faithful representation of the situation and follows the prescriptions of the foundational theory. This is expressed by Joseph E. Mayer in a unpublished book review for Wiley:<sup>6</sup>

I have a personal annoyance at the emphasis, so often made now, and here used [in the book], that we work with ‘models’. We know precisely the constituents of atoms and molecules, and since for most laboratory conditions the nuclear chemistry does not enter, we know the fundamental laws (quantum mechanics) that motivate the statistical mechanics of the systems with which we deal. Many of the results are independent of anything about which we have any doubt, other than the doubt which a scientist may have about anything. Why say we work with a ‘model’! To hell with that pussy [sic] footing! We work as close to reality as anyone works in any field of human endeavor.

Another possibility is that the model is known to be a less faithful description of reality, for instance by leaving out effects. However, if it can be argued that the effects left out do not matter, the model and these arguments will qualify as a theory. The reader should notice that the arguments for the validity of the model are counted as part of the theory.

So, the notion of a (phenomenological) theory is a multifaceted thing and includes various types of scientific accounts. However, here it will be used as a general and systematic treatment of a domain. The adjective ‘systematic’ implies that the treatment should be well-grounded in some respect. In contrast, a model is a specific representation of a phenomena or situation, which needs not be justified. However, as described above, a theory can consist of a model, but then the latter has to be well grounded.

## 2.2 Microscopic Modelling of Macroscopic Phenomena

This dissertation studies how insight into macroscopic phenomena is sought to be obtained through the use of models. More precisely, the phenomena under consideration are phase transitions, i.e., abrupt changes of the properties of a system as a result of changes in macroscopic parameters, e.g. temperature. A phase transition well-known from everyday

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<sup>6</sup>In Joseph Mayer Papers, Mandeville Special Collection, UC San Diego, Box 10, Folder 2.

life is the boiling of water, where  $\text{H}_2\text{O}$  goes from the liquid phase to the vapour phase. One type of phase transitions is of particular interest, so-called *continuous-phase transitions*. In such a phase transition the substance changes state without a jump in magnetisation, density, energy or similar quantities. In contrast, in a *first-order phase transition* there is a discontinuity in one of these quantities, for instance the latent heat associated with the boiling of water. The critical point of the liquid-vapour transition of water is a prototype of a continuous phase transition: The boiling temperature of water depends on the ambient pressure (the smaller the pressure, the lower the temperature). For pressures below 218 atmospheres and temperatures lower than  $374^\circ\text{C}$ , it is possible to differentiate the two phases from each other. However above these values of pressure and temperature, there will only be a single phase of high density. Furthermore, the fluid of this phase has peculiar properties, for instance the otherwise colourless water is milky at  $p = 218$  atmospheres and  $T = 374^\circ\text{C}$ . So, this pair marks a phase transition with qualitatively new properties and consequently it is called a critical point. The behaviour at or in the neighbourhood of the critical point – or more generally the point where the continuous-phase transition occurs – is called *critical phenomena*. In the 1960s similarities between various physical systems exhibiting such critical phenomena were realised.

The present dissertation studies attempts to gain insight into such critical phenomena by the use of models. There are two fundamentally different approaches to the thermal properties of physical systems in general and to those of phase transitions in particular: a macroscopic and a microscopic. The latter attempts to explain macroscopic properties on a molecular basis. The macroscopic approach, in contrast, employs thermodynamics “to deduce as much as we can about a change of state without assuming anything at all about the *mechanism* responsible for it.”<sup>7</sup> The programme of the microscopic approach is, in general terms, to “proceed from an assumed form of intermolecular interaction to predictions of the thermodynamic properties of an assembly by a mathematically rigorous argument.”<sup>8</sup> The vehicle for this procedure is (equilibrium) statistical mechanics. The microscopic approach has the following advantages over the macroscopic one:

The problem of the explanation of phase transitions on a molecular basis is among the most challenging facing the present statistical theory of matter. The special value of a statistical theory is that in principle it can predict both the nature of the phases and of the phase transitions from molecular properties. Such a theory, even if not perfectly accurate quantitatively, is clearly more effective in advancing our understanding than a purely thermodynamical one where we must assume the existence and characteristics of the two phases *ab initio*. From the standpoint of statistical mechanics, phase transitions are generally regarded as the result of cooperative interaction between molecules, and the great difficulty in the field lies in the complexity of the mathematical description of the simultaneous cooperation of many molecules. (Zimm et al.; 1953, p. 207)

During the epoch under study, there was widespread consensus that in order to understand physical phenomena, the approach has to be microscopic. Consequently, microscopic models, usually called statistical mechanical models, occupied a prominent position.<sup>9</sup> I shall

<sup>7</sup>Temperley (1956), pp. 3-4, emphasis in original.

<sup>8</sup>Temperley (1956), p. 2.

<sup>9</sup>This prominent position of statistical mechanical models was not something characteristic of critical phenomena only. Rather, it was shared by most physicists working on solid state physics.

restrict my attention to statistical mechanical models and only take thermodynamical considerations into account when they played a role in the endeavour to understand critical phenomena.

Microscopic modelling of macroscopic phenomena can serve two fundamentally different purposes: either to learn something about the *microscopic* constituents from which the model is built or gain insight into the *macroscopic* phenomena portrayed by the model.<sup>10</sup> The focus here will be restricted exclusively to the latter purpose, that of gaining insight into macroscopic phenomena. I am trying to uncover differences between various approaches to this task, but it seems reasonable to start with pointing out the common ground of these approaches.

There were some misgivings in the 1930s as to whether the formalism of statistical mechanics can in fact accommodate phase transitions. This formalism builds on the partition function which is a sum of analytic functions, while a phase transition is reflected in a non-analyticity of the thermodynamic functions. The solution to this problem was provided by H. A. Kramers in 1937, who argued that one needs to go to the so-called thermodynamic limit of infinite systems.<sup>11</sup> With Lars Onsager's solution of the Lenz-Ising model in 1944 it became crystal clear that equilibrium statistical mechanics is in fact able to accommodate phase transitions and the misgiving vanished.

Once the interaction energy between the molecular constituents of the model is known, then the macroscopic properties can in principle be derived from the microscopic model by applying statistical mechanics. In his famous dictum of 1929, P. A. M. Dirac said that quantum mechanics was in a state where it could provide the sought after interaction energy:

The general theory of quantum mechanics is now almost complete [...] The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation. (Dirac; 1929, p. 714)

So, according to Dirac, the foundational theory on which to base microscopic modelling, was known by the end of 1920s. The advent of the new quantum mechanics created a unique situation in physics where the existence of a foundational theory meant that there was consensus as to how the components *in principle* ought to behave.

Microscopic modelling takes a lot of things for granted: the masses of the constituents, the charge of the electrons, the origin of their spins and the values of these spins, etc. Furthermore, the conditions within the atomic nucleus is deemed insignificant for the modelling.

The above remarks can be summarised into what I venture characterises the consensus view of physicists and chemists during the time studied in this dissertation (from 1920

<sup>10</sup>The initial interest, for instance, of the American physicist Edmund Stoner in models of magnetism based on quantum mechanics was directed by the idea of obtaining information about the structure of atoms from magnetic properties. Later, however, Stoner (along with other physicists) became interested in learning about macroscopic magnetic properties *per se* from such models. See Keith and Qued c (1992)

<sup>11</sup>Brush (1983), pp. 246-247.

to 1971). Microscopic modelling of macroscopic phenomena in principle involves four fundamental steps:<sup>12</sup>

1. Selection of the components of the system (atoms, electrons, etc.).
2. Determination of the behaviour of the components (their interaction, whether they move, etc.).
3. Solution of the statistical mechanical equations derived from steps 1 and 2.
4. Comparison of the results of step 3 with experimental results.

Even though, as noted above, there were some misgivings about the applicability of statistical mechanics, it was in fact used, also prior to the solutions by Kramers and Onsager.

The advent of the new quantum mechanics meant that in principle it was possible to do step 2 on the basis of a theory and make models from first principles. However, *in practice* this was not possible because the applications of these principles lead to great mathematical intricacies, as already noted by Dirac in the quotation above. This means that it is always necessary to introduce some sort of additional abstraction, idealisation or approximation, which cannot be derived from first principles. For instance, based on the quantum mechanical theory of electron spin, Heisenberg could create a theory of ferromagnetism for the interaction between such spins. However, this theory did not follow directly from the first principles of quantum mechanics because he had to introduce some further assumptions. For gases, it was even more difficult to derive the interaction between the gas molecules or atoms.<sup>13</sup> So, it was far from practically possible to carry out step 2 from first principles. Hence nonquantum mechanical assumptions had to be introduced.

In fact, by the late 1930s it was well-known that mathematical difficulties place considerable constraints on what effects can be taken into account in a model and on how they are represented. So, throughout most of the time at issue in this dissertation, the circumvention of mathematical problems was perceived as a fundamental condition of modelling. This affected how phenomena are being modelled, as expressed nicely by Mark Kac in 1971:

Since the detailed nature of interactions in real physical systems is usually not known and since even the most far reaching simplifications still lead to enormous mathematical difficulties we must, in our attempts to understand

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<sup>12</sup>Here I have been inspired by Mogens Niss, who have described the full process of constructing a mathematical model in terms of the following steps.

At a minimum, it comprises (a) identifying the features of reality which are to be modelled; (b) selecting the objects, relations, and so on relevant to this end; (c) idealising them into shapes suitable for a mathematical representation; (d) choosing a mathematical universe to hold the model [...]; (e) performing a translation from reality to mathematics; (f) establishing mathematical relations between the translated objects, accompanied by assumptions and properties; (g) using mathematical methods to obtain mathematical results and conclusions; and (h) interpreting these as results and conclusions concerning the original area. In addition the process may include (i) assessing the model of confronting it with reality (e.g. observed or predicted data), by comparing it with other models, by relating it to established theory; and finally: (j) building if necessary, a new or modified model, thus running through the stages (a)-(j) once again. (Niss; 1989, p. 28)

<sup>13</sup>See Brush (1983), pp. 204-232 for an account of the time after the advent of quantum mechanics.

phase transitions, rely upon a narrow class of models which are balanced (precariously!) between realism and solubility.(Kac; 1971, p. 23)

This introduces a degree of freedom for the individual physicist in the modelling process, so there is no canonical way of modelling a particular phenomenon. This freedom is what makes modelling special and discriminates it from ‘applied quantum mechanics,’ and it is simply not possible to perform the programme of modelling a system solely from first principles. However, at least for the cases dealt with in this dissertation, quantum mechanics allowed an assessment of the validity of these assumptions and enabled a ranking of the various models.

So, in this situation models, in a phrase of Frigg and Hartmann (2005), step in “when theories are too complex to handle.”<sup>14</sup> They continue:

Theories may be too complicated to handle. In such cases a simplified model may be employed that allows for a solution [...]. Quantum electrodynamics, for instance, cannot easily be used to study the hadron structure of a nucleus, although it is the fundamental theory for this problem. To get around this difficulty physicists construct a tractable phenomenological model (e.g. the MIT bag model) that effectively describes the relevant degrees of freedom of the system under consideration (Hartmann 1999). A more extreme case is the use of a model when there are no theories available at all. (Frigg and Hartmann; 2005, p. 10)

It is the one of the themes of the present dissertation to examine different approaches to the handling of this situation.

## 2.3 Modelling Terminology

The notion ‘model’ will refer to the collection of components and their behaviour mentioned in steps 1 and 2 above. The formalism of the model is the statistical mechanical equations of step 3, which is based on the previous steps and can be used to derive consequences of the model. When the model is said to display, say, a Curie point, it is because something mimicking such a point occurs in the formalism. The demarcation of the notion of model implies that the same mathematical equations can be implicated in different models. This is the case for the Lenz-Ising model where the equations can describe different, but mathematically equivalent, models representing alloys, ferromagnets and gases, for instance. In such cases the term the Lenz-Ising model of alloys will be used and this model is distinguished from the Lenz-Ising model of ferromagnets.

So, to me the entity ‘model’ stops with the specification of the components and their behaviour, but others include more aspects in the notion of model. The philosopher Stephan Hartmann, for instance, considers what he calls a story to be part of the model. The story told by the model puts the model in a context but is not related to the components or formalism involved. I prefer to distinguish between a model and the story it tells, mainly because this allows to discuss different perceptions of the same model; in Hartmann’s definition this seems not to be possible.

<sup>14</sup>Frigg and Hartmann (2005), p. 3. Hartmann (1995) and Hartmann (1999) have another terminology for the same problématique.

### 2.3.1 The Perception of a Model

I wish to distinguish between the perception of a model and the use of it. The *perception* of model concerns the perception of the model in its capacity as a model, that is how well the model represents a particular situation or phenomenon. This is influenced by a host of factors, for instance the extent to which it agrees with experimental results or how well the model can be justified theoretically. The *role* of the model, on the other hand, concerns the function assigned to the model in a larger picture: What kind of insight is the employment and manipulation of the model thought to give? As noted below, models can play many different roles. Of course, which particular role a model is allowed to play in a given context depends on the perception of the model.

One aspect of the model perception is particularly important, namely the *realism* of the model. I would like to formalise the physicists' notion of realism (rather than that of philosophers). Even though it is not possible to derive everything from the foundational theory, this theory still constraints the modelling process through the realism of the model. Physicists often describe a model as more or less realistic and compare the realism of two models. What they seem to refer to with this adjective is the relation between the model and the world: The model is realistic if it faithfully portrays the system in question, that is take all or almost all of the features of the system into account and represent them in reasonable agreement with the foundational theory. However, since a model, by its very definition, always represents some aspect of the modelled situation in an unfaithful way, it is never perfectly realistic.

It is easiest to characterise the realism of a model in negative way, namely as the lack of simplifications. One should differentiate between three ways in which a model can be less than perfectly realistic: the cause of an idealisation or an abstraction. Margaret Morrison gives suitable definitions: "An idealisation is a characterisation of a system or entity where all its properties are deliberately distorted in a way that makes them incapable of accurately describing the physical world."<sup>15</sup> A case in point is the electron as a point particle. Abstraction Morrison defines as "a representation that does not include all of the systems properties, leaving out features that the system has in its concrete form."<sup>16</sup> The omission of intermolecular forces in the ideal gas model is an example of an abstraction. Both idealisation and abstraction can pertain either to the way the real system is supposed to be or our theoretical perception of it. In the epoch discussed here, quantum mechanics provided the ground for determining the behaviour of the components of the models, thereby giving a tool for assessing the degree of idealisation or abstraction for a given model. A third way in which a model can be less realistic is because an *approximation* is applied. In contrast to idealisation and abstraction, this simplification arises within the *mathematical* context. For instance, the equations of a model are made simpler by discarding terms or by introducing, say, the first few terms of a series expansions. By the term 'realism of a model' I will mean how well the model is thought to represent the real situation as described above, but it is easiest to determine the degree of realism negatively, as lack of idealisations, abstractions and approximations in the model. As noted above, I believe this captures the essence of the physicists' notion.

It should be realised that in this definition, realism of a model has nothing to do with whether or not the model agrees with experiments; that is another feature of the model. This feature is called *empirical adequacy*, following Cushing (1994). He wrote: "*Empirical*

<sup>15</sup>Morrison (1999), p. 38.

<sup>16</sup>Morrison (1999), p. 38.

*adequacy* consists essentially in getting the numbers right, in the sense of having a formula or an algorithm that is capable of reproducing observed data.”<sup>17</sup> However, I will extend this definition to include the ability to getting the *qualitative* features right, for instance by displaying something resembling a phase transition, but not necessarily quantitatively right.

There is a plethora of different types of models,<sup>18</sup> but only three which are of particular importance to the present will be characterised here. In his textbook on critical phenomena Nigel Goldenfeld has put it nicely:

There are two diametrically opposing views about the way models are used. The ‘traditional’ viewpoint has been to construct a faithful representation of the physical system, including as many of the fine details as possible. In this methodology, when theory is unable to explain the results of an experiment, the response is to fine-tune the parameters of the model, or to add a new parameter if necessary. An example of a branch of science where this is considered appropriate is quantum chemistry. On the other hand, such fine detail may actually not be needed to describe the particular phenomenon in which one is interested. Many of the parameters may be irrelevant, and even more importantly, the directly measurable quantities may well form dimensionless numbers, or even universal functions, which to a good approximation do not depend on microscopic details. (Goldenfeld; 1992, pp. 32-33)

The second point of view is that taken in the modern theory of critical phenomena.

The models employed in the second are well-known in physics, sometimes as minimal models, sometimes as *caricature* models.<sup>19</sup> I stick to latter usage, which seems to be coined by Yakov I. Frenkel. Michael E. Fisher has given an interesting discussion of such models:

We may well try to simplify the nature of a model to the point where it represents a ‘mere caricature’ of reality. But notice that when one looks at a good political cartoon one can recognize the various characters even though the artist has portrayed them with but a few strokes. Those well chosen strokes tell one all one really needs to know about the individual, his expression, his intentions and his character. So, accepting Frenkel’s guidance, [...] a good theoretical model of a complex system should be like a good caricature: It should emphasize those features which are most important and should downplay the inessential details. (Fisher; 1983, p. 47)

For instance, if a system modelled involves spins, one should only retain those features of the spins that are needed to reproduce the essential features of the real system; whether a full quantum mechanical description is necessary or a classical one will do the job, is only decided by a test of the latter’s ability to reproduce the interesting traits.

A caricature model will usually attempt to uncover what mechanisms are responsible for a particular feature of the phenomenon in question.

<sup>17</sup>Cushing (1994), p. 10, emphasis in the original.

<sup>18</sup>For a number of those recognised by philosophers of science, the reader may consult Frigg and Hartmann (2005).

<sup>19</sup>Minimal model is the terminology of Goldenfeld (1992) and Batterman (2002). The latter subscribed to the use of the former, which defined minimal model as the “model which most economically caricatures the essential physics”(Goldenfeld; 1992, p. 22). Strictly speaking, a caricature model need not be the *most* economical model, but I think that the notions of caricature model and minimal model essentially try to capture the same aspect of models, namely the focus on a few features.

A third type of models to consider is *toy models*, also called study models or probing models:

These are models which do not perform a representational function and which are not expected to instruct us about anything beyond the model itself. The purpose of these models is to test new theoretical tools that are used later on to build representational models. In field theory, for instance, the so-called  $\phi^4$ -model has been studied extensively not because it represents anything real (it is well-known that it doesn't) but because it allows physicist [sic] to 'get a feeling' for what quantum field theories are like and to extract some general features that this simple model shares with more complicated ones [...]. (Frigg and Hartmann; 2005, p. 11)

So, toy models differ from caricature models with respect to their ability to represent a real systems: the latter model may be a caricature of the system, but it is supposed to portrayed nonetheless; this is not the case for the former model.

### 2.3.2 The Role of a Model

I now turn to some general remarks about the roles models can play. One fundamental distinction is whether the overall purpose of the modelling enterprise is to describe and/or predict, on the one hand, or, on the other, to prescribe.<sup>20</sup> The former, which is more or less self-explanatory, aims at capturing or understanding aspects of some entity. The latter seeks to provide grounds for making decisions or taking actions in situations where it is not practically desirable or possible to 'experiment' with the system in the real world, for instance because it is too expensive or dangerous. The construction of a bridge is such a situation where it is sensible to model the bridge prior to construction.

The models considered in this dissertation are of the first kind only. However, such models can still have numerous functions in science. Hartmann (1999) mentions a few: A model can a) apply a foundational theory; b) test a theory; c) develop a theory; d) replace a theory; e) explore the features of a theory; f) help gain understanding. However, as Hartmann writes, this is far from an exhaustive list.

These distinctions are based on the purpose of the modelling *enterprise*. It is usually not possible to determine the function of the model by looking at the model *per se* (the components and formalism involved) from this enterprise. A model will typically tell a *story*, to use one of Hartmann's notions, which is detached from the formalism and components of the model, and one needs to have access to the story to see the function of the model. The story told by the model puts it in a context.

A story is a narrative told *around* the formalism of the model. It is neither a deductive consequence of the model nor the underlying theory. (Hartmann; 1999, p. 344)

The story refers to the objects of the model or theory<sup>21</sup> and "the story fits the model in a larger framework (a 'world picture') in a non-deductive way."<sup>22</sup> Moreover, a story is "an

<sup>20</sup>The description of this distinction builds on a paper by my father Mogens Niss (2005b).

<sup>21</sup>Hartmann discusses attempts at understanding foundational theories rather than macroscopic phenomena, but I believe his ideas can be transferred to the latter case.

<sup>22</sup>Hartmann (1999), p. 344.



integral part of a model; it complements the formalism. To put it in a slogan: *a model is an (interpreted) formalism+a story.*<sup>23</sup> As pointed out by Hartmann this notion can be used to accommodate a view of models where their function is not only a matter of empirical adequacy and logical consistency, but also of whether the model is able to tell a plausible story.<sup>24</sup>

I think one can distinguish between two fundamentally different approaches to how models function. In the ‘traditional’ approach one is interested in a particular situation in the real world. This situation is represented by a quite realistic model. An example could be a pendulum where Newtonian mechanics can be applied to an idealisation of the pendulum – a model. The model can be successively refined to take a number of correction terms into account and the refined model is the end goal. In the second approach, one also models a physical phenomenon. The foundational theory does provide some guidelines for how the components and their behaviour should be modelled, but the modelling involves many unjustified assumptions and the model is far from theory-driven. More importantly, the situation is so complicated that the model is not a faithful representation of the macroscopic phenomenon in question. So, there is a need for a new kind of theorising and this is based on the model or a number of models. This theorising, hopefully, leads to a theory of the physical phenomenon. In this case, the model in itself is not the end goal, but the theory which can be build from it and similar models. In large parts of the development under consideration, the second approach was taken and models took part in the building of a theory of a macroscopic phenomenon.

## 2.4 Explanation and understanding

What constitute explanation and understanding in science is a recurrent theme in the philosophy of science. I shall not go deeply into the this literature, as my interest is in what *scientists* put into those terms and possible changes of the meanings of those terms over time. However, I believe the scientists’ use is an elaboration of the vernacular of, say, the Oxford English Dictionary. One among several definitions in OED of “explain” that captures the physicists’ parlance is “To make plain or intelligible,” while the analogous entry for “to understand” is “To comprehend; to apprehend the meaning or import of; to grasp the idea of.”

On the terminological level, there seems to be consensus, from the 1920s and onwards about what an explanation of a macroscopic phenomena means. For these scientists, to explain a phenomenon is to provide a microscopic model and show that it reproduces the features of the phenomenon in question. So, the Heisenberg model explains the Curie point of ferromagnets because the model displays a temperature similar to the Curie temperature of real ferromagnets. Most of the actors mentioned in this dissertation considered the realism of the model to be irrelevant to its explanatory power. For instance, Lenz and Ising explicitly considered a previous account by Pierre Weiss to be only formally satisfactory, but not theoretically. Yet, both of them described this account as an “explanation” because it was capable of reproducing the Curie temperature.

In contrast, it is not possible to give an operational definition of the term “understanding” that all the scientists would agree on. Some would not distinguish between

<sup>23</sup>Hartmann (1999), p. 344.

<sup>24</sup>Hartmann stresses that the story helps us obtain understanding of the physical mechanisms, but unfortunately he does not elaborate on how this is done.

understanding and explanation, while others say that a phenomenon is understood if it is possible to reproduce its features from first principles. Still others hold the view that if the properties of the phenomenon can be predicted from a microscopic model, the phenomenon is understood. I do not go any further into this question here, which is in fact one of the central issues of the dissertation and will consequently be dealt with along the way.



## **Part I**

# **The Birth of the Lenz-Ising Model: 1920–1950**



# 3

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## Introduction to Part I

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This part of the dissertation serves four different purposes. The first is to provide information relevant for the entire dissertation: the part introduces the Lenz-Ising model, states important technical results on the model (for instance, Lars Onsager's solution of the two-dimensional case) and describes other models relevant for the remainder of the dissertation.

The second purpose is to supply the first chapter of the history of the Lenz-Ising model. It charts the early history of the model from it was proposed in the early 1920s by W. Lenz and E. Ising as a model of ferromagnetism, over the contemporary physicists' rejection of the model as a credible representation of ferromagnetism to its rise within so-called transition points of cooperative phenomena in the 1940s and the 1950s. This part therefore concerns the time from the 1920s to 1950, including the origins of the model.

The third purpose of the present part is to contribute to the answering of the central questions of section 1.1. More precisely, the part addresses two questions. Firstly, what was the effect of the replacement of the old quantum theory with the new quantum mechanics? Secondly, why did the model survive this replacement in view of the dismissive attitude towards it as a representation of ferromagnetism?

Finally, this part lays the ground for my discussion of the other central questions of the dissertation by showing what role the model was allowed to play prior to the 1960s.



# 4

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**Paper:**  
**“History of the Lenz-Ising Model  
1920–1950”**  
**(Archive for History of Exact Sciences)**

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## *History of the Lenz-Ising Model 1920–1950: From Ferromagnetic to Cooperative Phenomena*

MARTIN NISS

*Communicated by* R. H. STUEWER

### **Abstract**

I chart the considerable changes in the status and conception of the Lenz-Ising model from 1920 to 1950 in terms of three phases: In the early 1920s, Lenz and Ising introduced the model in the field of ferromagnetism. Based on an exact derivation, Ising concluded that it is incapable of displaying ferromagnetic behavior, a result he erroneously extended to three dimensions. In the next phase, Lenz and Ising's contemporaries rejected the model as a representation of ferromagnetic materials because of its conflict with the new quantum mechanics. In the third phase, from the early 1930s to the early 1940s, the model was revived as a model of cooperative phenomena. I provide more detail on this history than the earlier accounts of Brush (1967) and Hodderson, Schubert, Heims, and Baym (1992) and question some of their conclusions. Moreover, my account differs from these in its focus on the development of the model in its capacity as a *model*. It examines three aspects of this development: (1) the attitudes on the degree of physical realism of the Lenz-Ising model in its representation of physical phenomena; (2) the various reasons for studying and using it; and (3) the effect of the change in its theoretical basis during the transition from the old to the new quantum mechanics. A major theme of my study is that even though the Lenz-Ising model is not fully realistic, it is more useful than more realistic models because of its mathematical tractability. I argue that this point of view, important for the modern conception of the model, is novel and that its emergence, while perhaps not a consequence of its study, is coincident with the third phase of its development.

### **Introduction**

Judging by the number of research papers published on the Lenz-Ising model since 1940, it is one of the most studied models in modern physics. Its greatest success during the last half century has been in the study of phase transitions,<sup>1</sup> but it also has been applied to a wide range of physical phenomena. It is discussed today in virtually every

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<sup>1</sup> See, for example, Domb (1996).

modern textbook on statistical mechanics. Because of its ubiquity and importance in modern physics, a historical study of its origin and development is merited.

More generally, a historical study of the Lenz-Ising model will shed light on the use of models in physics. As in all aspects of science, opinions concerning a particular model change both with time and across the scientific community. Some may think that a given model is a useful and realistic representation of a physical phenomenon, while others may reject it because, for instance, it is at odds with fundamental theories. The history of the Lenz-Ising model presents a good opportunity to study such changes in attitude towards a model. It can be viewed as a characteristic example of a certain class of physical models, simple statistical-mechanical models, which also include such models as the Heisenberg model, the Potts model, and the spherical model, all of which play important roles in modern physics. The Lenz-Ising model thus is not a marginal “pathological” case. Moreover, as its theoretical basis changed with the emergence of the new quantum mechanics, it underwent great changes with respect to the phenomena it represents, its physical realism, and the insights it provided.

One particular aspect of the history of the Lenz-Ising model stands out and is related to the primary reason for its ubiquity in modern physics: It strikes a balance between physical nonrealism and realism. That is to say, the Lenz-Ising model usually is considered to be a very crude model of the phenomena it is assumed to represent, but at the same time it is able to capture some of their essential features. Its simplicity, moreover, makes it amenable to mathematical treatment (at least in one and two dimensions). Thus, Kerson Huang remarked in 1963:

The Ising model is a crude attempt to simulate the structure of a physical ferromagnetic substance . . . . Its main virtue lies in the fact that a two-dimensional Ising model yields to an exact treatment in statistical mechanics. It is the only nontrivial example of a phase transition that can be worked out mathematically.<sup>2</sup>

This emphasis on its mathematical tractability at the expense of its physical realism seems to be characteristic of statistical-mechanical models after World War II. As Mark Kac noted in 1971:

Since the detailed nature of interactions in real physical systems is usually not known and since even the most far reaching implications still lead to enormous mathematical difficulties we must, in our attempts to understand phase transitions, rely upon a narrow class of models which are balanced (precariously!) between realism and solubility.<sup>3</sup>

This attitude toward statistical-mechanical models of phase transitions, including the Lenz-Ising model, seems to have emerged around World War II and since then has become widespread among physicists. I will trace the emergence of this new attitude towards physical models between 1920 and 1950 in the special case of the Lenz-Ising model.

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<sup>2</sup> Huang (1963), p. 329.

<sup>3</sup> Kac (1971), p. 23.

Ernst Ising (1900–1998) and the history of the Lenz-Ising model have been subjects of earlier studies.<sup>4</sup> Stephen G. Brush (1967),<sup>5</sup> in a seminal article, traced the history of the Lenz-Ising model between 1920 and 1967, concentrating on its *mathematical* results. Hodderson, Schubert, Heims, and Baym (1992), in their history of it in the context of collective phenomena,<sup>6</sup> discussed its *physical* aspects, but only briefly. I will give a more detailed account of its early history and focus on its evolution as a *model* by charting its development with respect to three of its aspects: (1) its degree of physical realism, that is, how faithfully physicists believed that it represented physical phenomena; (2) the reasons that physicists investigated and used it; and (3) the changes in its theoretical basis following the creation of the new quantum mechanics in 1925. I will assume no prior knowledge of its history and will not discuss its mathematical aspects, since they have been treated elsewhere<sup>7</sup> and play a minor role in my account.

Regarding terminology, I use the term “realism” in connection with a model to represent the extent of its agreement with a physical phenomenon. One way to measure this agreement is to consider its degree of idealization, where I subscribe to Margaret Morrison’s definition:

An idealisation is a characterisation of a system or entity where its properties are deliberately distorted in a way that makes them incapable of accurately describing the physical world. By contrast, an abstraction is a representation that does not include all of the systems [*sic*] properties, leaving out features that the systems [*sic*] has in its concrete form. An example of the former is the electron as a point particle and the latter is the omission of intermolecular forces from the ideal gas.<sup>8</sup>

By this definition, the less idealizations of a model, the higher its degree of realism. I believe that this definition is close to physicists’ use of the term, for example, by Kac above.

I also must remark on the appellation, the Lenz-Ising model. Physicists almost exclusively call it the Ising model, even though Lenz contributed significantly in proposing it. Brush (1967), however, followed Ising’s own recommendation and called it the Lenz-Ising model, but had little success in changing its name among physicists. Mathematical physicists McCoy and Wu (1973), for instance, stuck doggedly to calling it the Ising model in their monograph on its two-dimensional variant, arguing that Lenz, in contrast to Ising, had not provided any computations. They admittedly acknowledge Lenz’s work but to me Lenz’s role in proposing the model seems at least as important as Ising’s relatively straightforward calculations, so I regard Brush’s name for it as more appropriate and accordingly will use it. Finally, I use the term “*n* dimensions” in the so-called *n*-dimensional Lenz-Ising model to refer to the dimensionality of the lattice on which the

<sup>4</sup> Biographical data of Ising can be found in Stutz and Williams (1999), Kobe (1997), and Kobe (2000). Ising changed his first name to Ernest when he became an American citizen in 1953.

<sup>5</sup> See also Brush (1983), which, however, does not contain new material about the model.

<sup>6</sup> Their study appears as a chapter in Hodderson, Braun, Teichmann, and Weart (1992), a pioneering book on the history of solid-state physics.

<sup>7</sup> Brush (1967).

<sup>8</sup> Morrison (1999), p. 38.

model “lives.” When I specify no dimension, I assume that the dimension of the lattice is arbitrary, in accordance with the terminology accepted today.

I see roughly speaking three phases in the development of the Lenz-Ising model. In the first phase, Lenz introduced one of the two basic assumptions of the model in 1920 and his student Ising introduced the other one in 1924. They proposed their model to give a theoretically more satisfactory account of experimental results for paramagnetism and ferromagnetism than Pierre Weiss had provided with his theory of magnetism, the dominant theory at that time. Lenz believed, as did Weiss, that magnetic materials consist of elementary micromagnets placed in a regular array, but Lenz, in contrast to Weiss, allowed each of these micromagnets to point in either of only two directions. Ising then carried out calculations on Lenz’s model by assuming only nearest-neighbor interactions between the micromagnets, finding that it did not display ferromagnetic behavior in one dimension. He concluded erroneously that this result also was valid in three dimensions.

During the second phase, from 1925 to 1936, the validity of Ising’s conclusion for the three-dimensional case was a subject of controversy. Moreover, the Lenz-Ising model was dismissed as a model of ferromagnetism, because it was incompatible with Heisenberg’s theory of ferromagnetism. It was studied, however, as a simple approximation to Heisenberg’s model. Then, in 1936, Rudolf Peierls showed that it does exhibit ferromagnetism in two dimensions. Further, a mathematically equivalent model also was investigated in other areas, such as in the theory of binary alloys and gas adsorption.

In the third phase, after 1936, several physicists realized that the description of sharp transition points of so-called cooperative phenomena — phenomena arising in systems in which the cooperation of its constituent units is of fundamental importance — pose enormous mathematical problems.<sup>9</sup> The way around them was to study very simple models of cooperative phenomena in which the emphasis was on mathematical tractability rather than on physical realism. For example, H.A. Kramers and G.H. Wannier used the Lenz-Ising model in their theory of ferromagnetism even though they recognized that it was an unrealistic representation of ferromagnetism. They conjectured that the specific heat as a function of temperature for the two-dimensional model shows a singularity when the temperature approaches a certain value. Lars Onsager, in an attempt to understand transitions with no release of latent heat, proved their conjecture in 1944. The work of Kramers and Wannier and Onsager precipitated a flood of publications on the Lenz-Ising model whose focus was on the general properties of transition points in a wide range of physical systems rather than on the particular features of a given system.

### Physics preliminaries

Most physicists today view the Lenz-Ising model as a mathematical structure that can represent a variety of different physical phenomena. For concreteness, I will define the model in this section in *modern* ferromagnetic parlance. Thus, the model lives on a

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<sup>9</sup> Cooperative phenomena are not the same as what was termed critical phenomena in the 1960s. Critical phenomena are cooperative phenomena, but the latter class includes phenomena that do not exhibit critical behavior.

lattice and a particle is assigned to each lattice site. The particle has an intrinsic angular momentum, its spin  $\sigma$ , which is restricted to point either up or down (and is typically represented by an arrow). A configuration of the model is a specification of the spin for each lattice site; for a two-dimensional lattice with, say,  $N \times M$  lattice sites, there are  $2^{NM}$  possible configurations. For example, one configuration for  $6 \times 4$  lattice sites can be visualized as follows:

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      ↑ ↓ ↓ ↑
      ↑ ↓ ↑ ↓
      ↓ ↑ ↑ ↓
      ↑ ↑ ↓ ↑
      ↑ ↑ ↓ ↑
      ↑ ↓ ↑ ↓

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Only particles that are nearest neighbors interact, that is, they have to be connected by exactly one bond on the lattice. If the spins of two nearest neighbors in the configuration have the same orientation (both either up or down), then this pair contributes an energy  $-J$  to the total energy. If they have opposite orientations, they contribute an energy  $J$ , the so-called *interaction* energy, which is the same for all pairs and is assumed to be positive for a ferromagnet (if  $J$  is negative, the model describes an antiferromagnet). Each particle (electron) has a magnetic moment  $\mu$  owing to its spin that couples with an external magnetic field of strength  $H$ , so that the energy associated with this coupling is  $\mu H \sigma_j$  for site  $j$ . The total energy  $E_i$  of a configuration  $i$  is thus given by

$$E_i = - \sum_{\langle n,m \rangle} J \sigma_n \sigma_m + \sum_j \mu H \sigma_j, \quad (1)$$

where the first sum is over all pairs of nearest neighbors and the second is over all lattice sites.

Suppose now that the energy of each configuration has been determined. According to a fundamental assumption of equilibrium statistical mechanics, the probability  $P_i$  that the system is in the configuration  $i$  with energy  $E_i$  is determined by this energy and is given by the so-called Boltzmann factor:

$$P_i = Z^{-1} \exp \left( -\frac{E_i}{kT} \right), \quad (2)$$

where  $k$  is Boltzmann's constant,  $T$  is the (constant) absolute temperature, and  $Z$  is the partition function; since the sum of the probabilities for all states has to equal 1

$$Z = \sum_i \exp \left( -\frac{E_i}{kT} \right). \quad (3)$$

Thus, since the total energy  $E_i$  depends on the external magnetic field  $H$  and the interaction energy  $J$ , the partition function  $Z$  depends on these quantities, as well as on the absolute temperature  $T$ .

In principle, equations (1–3) suffice to determine all of the macroscopic properties of the system. For instance, the average energy is given by

$$E = \sum_i E_i P_i. \quad (4)$$

Other quantities can be computed by taking suitable derivatives of the partition function  $Z$ . For instance, the magnetization  $M$  is defined by

$$M = kT \frac{1}{N} \frac{\partial \ln Z}{\partial H}. \quad (5)$$

In the Lenz-Ising model, this definition can be shown to be equivalent to another procedure that may appear to be more natural: For every configuration, compute the quantity

$$\frac{1}{N} \sum_i \mu \sigma_i, \quad (6)$$

and then average this quantity over all possible configurations; the result is the magnetization  $M$ .

A quantity of particular interest is the average magnetization  $M_0$  as a function of the absolute temperature when the external field tends to zero:

$$M_0(T) = \lim_{H \rightarrow 0} M. \quad (7)$$

If  $M_0(T)$  is nonzero, then the Lenz-Ising model is said to have a spontaneous magnetization and to be ferromagnetic at  $T$ , because this is analogous to the behavior of real ferromagnets. Historically, an important issue was whether or not a temperature  $T$  exists in the Lenz-Ising model (as well as other models of ferromagnetism) that mimicks the Curie temperature of real ferromagnets, which marks a transition from a low-temperature, ferromagnetic regime to a high-temperature, paramagnetic (nonferromagnetic) regime. Such a transition, which in mathematical terms is a singularity, can occur only in the thermodynamic limit in which the number of lattice sites tends to infinity. If the dimension of the lattice is greater than one, the computation of the partition function  $Z$  presents formidable mathematical difficulties in this thermodynamic limit. For the Lenz-Ising model, this computation has been done only for one and two dimensions, and in the latter case only for zero magnetic field. Strenuous efforts to extend these results have so far proven to be futile.<sup>10</sup>

### Models and theories of magnetism prior to Lenz and Ising

Lenz and Ising's purpose in introducing their model was to reproduce the properties of paramagnetic and ferromagnetic solids by applying statistical mechanics to micro-magnets. In this they relied on a long tradition of making such microscopic models (sometimes called theories) of magnetism, which I will summarize below, focusing on their microscopic, statistical, and quantum-mechanical aspects. First, however, I note a crucial experimental result that the French physicist Pierre Curie (1859–1906) reported in 1895.<sup>11</sup> Curie singled out three classes of magnetic substances, which today are called

<sup>10</sup> Cibra (2000). In fact, Cibra reports that it has been proven that the solution of the three-dimensional model in zero field is NP-complete.

<sup>11</sup> Curie's work is described in Keith and Quedec (1992), which contains more details than I give here.

diamagnetic, ferromagnetic, and paramagnetic substances and reported what is today called the *Curie law*, that the magnetic susceptibility  $\chi_T$  of a paramagnetic substance varies inversely with the absolute temperature  $T$ :

$$\chi_T \equiv \left( \frac{\partial M}{\partial H} \right)_T \propto 1/T, \quad (8)$$

where as before  $M$  is the magnetization and  $H$  is the strength of the external magnetic field.

Eckert, Schubert, and Torkar (1992, pp. 23–24) ascribe the emergence of microscopic models of magnetism in the second half of the nineteenth century to the earlier enunciation of the concept of the atom together with the long-established knowledge that fragments of a magnet are also magnetic. This led to the view that magnetic matter consists of a number of tiny magnetic needles, each of which represents an atom or molecule with a magnetic moment. Wilhelm Weber (1804–1891) put forward in 1852 the first important model based on this idea; he assumed that each atom or molecule is able to rotate freely around an axis.<sup>12</sup>

Keith and Quedec (1992) claim that Pierre Curie's student Paul Langevin (1872–1946) was the first to apply Boltzmann's statistical ideas in the field of magnetism in his theories of diamagnetism and paramagnetism of 1905. I will only discuss Langevin's theory of paramagnetism, drawing on his original paper and the account of it in Mehra and Rechenberg (1928a). Langevin assumed that the total magnetic moment  $M$  of the molecular micromagnets arises from the revolution of electrons in them and then employed Boltzmann's theory to a gas of such molecules in an external magnetic field of strength  $H$ .<sup>13</sup> If  $W$  is the difference in potential energy of a molecule between any two points in the gas, and if its magnetic moment is at an angle  $\alpha$  with the external magnetic field, he then found that  $W = MH \cos \alpha$  and the ratio of the density of the molecules between these two points is proportional to  $e^{-W/kT}$  or

$$\exp \left( -\frac{MH \cos \alpha}{kT} \right). \quad (9)$$

Using this result, Langevin then obtained his famous eponymous equation for the intensity of magnetization

$$I = MN \left( \frac{Cha}{Sha} - \frac{1}{a} \right), \quad (10)$$

where  $a = \frac{MH}{kT}$  and  $Ch$  and  $Sh$  are the hyperbolic cosine and sine functions, respectively.

<sup>12</sup> In a paper of 1890, Alfred Ewing described a “simulation” of Weber's model: Ewing built a large-scale version of Weber's model in two dimensions consisting of an array of concrete, macroscopic magnetic needles attached to a table. By placing this macroscopic physical model in a solenoid, Ewing could reproduce the essential features of the magnetization curve of iron; see Eckert, Schubert, Torkar (1992), pp. 24–25.

<sup>13</sup> Mehra and Rechenberg (1982a), pp. 423–424.

Pierre Weiss (1865–1940), another Frenchman who since 1902 was working at the Eidgenössische Technische Hochschule in Zurich,<sup>14</sup> made several important contributions to the theory of magnetism, including an extension of Langevin’s theory of paramagnetism to ferromagnetism (still restricted to isotropic materials), and a theory of magnetism of crystals. I will discuss Weiss’s latter theory later in connection with Lenz’s work and for the moment only outline his former theory, drawing on the accounts by Mehra and Rechenberg (1982a) and Keith and Quedec (1992).

One of Weiss’s most important ideas was his so-called “molecular-field hypothesis” (sometimes referred to as his “internal-field hypothesis”), which he defined as follows:

I assume that each molecule experiences, from the collection of molecules surrounding it, a force equal to that of a uniform field proportional to the intensity of magnetization and in the same direction.<sup>15</sup>

The total field affecting a molecule, which I will designate as  $H_{total}$ , is the sum of this internal-field and the external field,

$$H_{total} = NI + H. \quad (11)$$

where  $N$  is the number of molecules and  $I$  is the intensity of magnetization. Weiss preserved Langevin’s equation (10), but he replaced the external field  $H$  by  $H_{total}$ , and he concluded that if a molecular field is present, then there exists a characteristic temperature below which isotropic media exhibit a spontaneous magnetization, even in the absence of an external field  $H$ , and above which they do not. He later called this temperature the Curie point.

Weiss also was the first to apply quantum-theoretical considerations to the magnetic properties of matter,<sup>16</sup> which according to Mehra and Rechenberg (1982a, p. 424) initiated a new direction of research on paramagnetism. Thus, two Dutch physicists, E. Oosterhuis and W.H. Keesom, in 1913 and 1914, respectively, modified Langevin’s classical theory by replacing the energy  $kT$  with the average quantum-mechanical rotational energy of the molecular magnets, which enabled them to account for some of the discrepancies between Langevin’s classical theory and experiments. Their work stimulated that of others, for example, that of Jan von Weyssenhoff and Fritz Reiche, who by means of a number of refinements were able to achieve good agreement with experimental results for substances at still lower temperatures.<sup>17</sup>

Nevertheless, the German physicist Otto Stern (1888–1969) sharply criticized the basic assumptions underlying the above theories in 1920.<sup>18</sup> He pointed out that Weiss and his successors had applied Langevin’s theory to gases at temperatures so low that they would likely have crystallized and hence had implicitly assumed that the gas molecules, as the carriers of micromagnets, were as free to rotate in the solid phase as in the gaseous phase. This assumption, however, Stern went on, was clearly contradicted

<sup>14</sup> Keith and Quedec (1992), p. 374.

<sup>15</sup> Weiss (1907), p. 662, translated in Keith and Quedec (1992), p. 376.

<sup>16</sup> The results were published in Weiss (1911).

<sup>17</sup> Mehra and Rechenberg (1982a), p. 424.

<sup>18</sup> Stern (1920); Mehra and Rechenberg (1982a), pp. 431–432.



by the anisotropy characteristic of crystalline structure. Weiss actually had anticipated this objection and had tried to circumvent it in a paper of 1913 where he had shown that Curie's law follows from the assumption that the molecules are bound to fixed equilibrium positions whose orientations are in no preferred directions. Stern, however, pointed out a flaw in Weiss's calculations and, by using Boltzmann's formalism, showed that Weiss's assumption led to a much weaker dependence of the magnetic susceptibility on temperature than exhibited by Curie's law. Moreover, Stern did not attach much importance to the apparent agreement between the theories of Weiss's successors and experiments because their theories embodied several adjustable parameters.

By 1920, in sum, there was general agreement among physicists that magnetic materials consist of elementary micromagnets, and that Boltzmann's statistical formalism was the right tool to use to describe their magnetic properties theoretically. Weiss's theories of magnetism, and their subsequent modifications by others, were able to reproduce at least some of the experimental results, but they also faced criticism. Weiss's molecular-field hypothesis did not seem to be satisfactory, despite its empirical success, because it lacked a satisfactory physical explanation. More generally, the physical origin of the magnetic interaction was of great concern at the time. Further, Weiss's approach required clarification because of his assumption of the free rotatability of the molecular magnets in solid materials, which therefore had to be modified, first according to Otto Stern and now according to Wilhelm Lenz.

### Lenz's paper

Wilhelm Lenz (1888–1957) *promovierte* in 1911 under Arnold Sommerfeld at the University of Munich with a dissertation on electrodynamics (on the capacitance, resistance, and self-inductance of coils) and continued this work as Sommerfeld's assistant, completing his *Habilitationsschrift* in 1914 (on eigenoscillations in coils).<sup>19</sup> He was appointed as *ausserordentlicher Professor* at the University of Rostock in 1920, where he worked on various subjects (for example, proposing a theory of molecular band spectra<sup>20</sup>) before turning to the theory of magnetism.<sup>21</sup>

His contribution to the Lenz-Ising model was the only paper he published on microscopic theories of paramagnetism and ferromagnetism. This digression may have been inspired by Stern's paper, which he cited in his own paper. In fact, Lenz may have met Stern personally in Berlin in April 1920, since they both attended a lecture that Niels Bohr gave then at a meeting of the German Physical Society. Lenz presented his work five months later at the 86th *Naturforscherversammlung* in Bad Nauheim, which took place from September 19–25, 1920,<sup>22</sup> and published it later that year as a paper entitled "A Contribution to the Understanding of Magnetic Phenomena in Solid Materials."<sup>23</sup>

<sup>19</sup> Sommerfeld (1948), p. 186, attested that the replacement of Debye with Lenz as his assistant in 1911 caused him no doubts.

<sup>20</sup> Sommerfeld (1948), p. 186.

<sup>21</sup> Mehra and Rechenberg (1982a), p. 334; Brush (1967), p. 885.

<sup>22</sup> Mehra and Rechenberg (1982a), p. 804.

<sup>23</sup> Unless stated otherwise all translations are my own.

To Lenz, the main magnetic phenomenon that demanded understanding was the Curie law of paramagnetism, which Heike Kamerlingh-Onnes (1853–1926) and Oosterhuis had confirmed experimentally for a number of salts at low temperatures. Lenz argued that because this law is so fundamental, by extension “the key to understanding the very complicated ferromagnetic phenomena ought to lie here,”<sup>24</sup> their most prominent aspects being the temperature dependencies of both the susceptibility and the spontaneous magnetization. Nevertheless, despite his general approach, he focussed mainly not on ferromagnetism but on paramagnetism, which he treated quantitatively. Most of his successors thus saw his paper as falling in the domain of paramagnetism,<sup>25</sup> with one notable exception, namely Arnold Sommerfeld, who remarked in a note written on the occasion of Lenz’s 60th birthday that:

Very early [in 1920] Lenz had pointed to the magnetic turnover processes in solid paramagnetic materials in order to explain the Curie law, with an outlook to ferromagnetism.<sup>26</sup>

Throughout his paper, in fact, Lenz stressed the connection between paramagnetism and ferromagnetism, and, as we shall see, he derived the fundamental assumptions of his theory from observations not of paramagnetic but of ferromagnetic materials, so he evidently considered the two types of magnetism to arise from the same basic mechanism. He did not express this idea explicitly, however.

As noted above, Lenz regarded Weiss’s theories of paramagnetism and ferromagnetism as insufficient, because he endorsed Stern’s criticism of them that the elementary magnets cannot rotate freely in a solid. Moreover, to Lenz the molecular-field (or “self-field”) hypothesis, “offers only a purely phenomenological hint”<sup>27</sup> about how to explain ferromagnetism. Nonetheless, he embraced some of Weiss’s basic assumptions that magnetic materials contain small magnetic needles but began to rethink their ability to rotate:

To obtain the Curie law, the assumption of free rotatability of the magnets thus seems indispensable; and since the crystal structure prohibits free rotation of the molecules, one might think of free rotatability of the atoms. However, this assumption, too, is incompatible with our conception of the crystal structure, since we, following Born, must assume that the symmetry of the crystals is already preformed according to the structure and spatial position of those atoms.<sup>28</sup>

What Lenz meant by “preformed” is not clear, but he may have meant that the atoms determine the structure and hence the symmetry of the crystal, which is consistent with the interpretation that Max Born gave in his influential monograph, *Dynamik der Kristallgitter*, of 1915,<sup>29</sup> where he claimed that atoms, not molecules, are the building blocks of crystal lattices. Further, he assumed that the chemical forces that keep the atoms in place

<sup>24</sup> Lenz (1920), p. 613.

<sup>25</sup> See, for example, Ehrenfest (1921), p. 793; Kramers (1929), p. 25; and Kramers and Becquerel (1929), p. 49.

<sup>26</sup> Sommerfeld (1948), p. 186.

<sup>27</sup> Lenz (1920), p. 613.

<sup>28</sup> *Ibid.*, p. 614.

<sup>29</sup> Born (1915), pp. 1–2.

in a crystal are identical to those that act between atoms in liquids and gases. Lenz thus may have taken Born to mean that the atoms in a crystal are responsible for its spatial characteristics.

Proposing a new notion of free rotatability “adjusted to the crystal structure,”<sup>30</sup> Lenz cited experimental results on pyrrhotite and magnetite for temperatures where they are ferromagnetic, not paramagnetic. Weiss had concluded that the basic unit of pyrrhotite is a hexagonal prism that can be magnetized only in its magnetic plane, that is, its hexagonal base.<sup>31</sup> Lenz now declared:

As is well known, it is a property of the crystal state of the minerals mentioned to be magnetized to spontaneous saturation. It is not in practice possible to change the magnetization of the sample to a noticeable degree by applying an external [magnetic] field, but the orientation of the magnetization can be changed, since the crystal symmetry of magnetite corresponds to a turnover [*ein Umklappen*] for each  $90^\circ$ , and for pyrrhotite a turnover for each  $60^\circ$  is observed . . . . Thus, for the orientation of the elementary magnets there are always several equal positions determined by the crystal symmetry . . . and one may assume in general that for every position at least its opposite is equal to it. Since free rotatability of the elementary magnets therefore has to be refuted, it can be concluded from the above that they have the ability to turn over. I want to show that this assumption is sufficient to explain the Curie law.<sup>32</sup>

A reasonable interpretation of Lenz’s turnover argument is that the structure of the crystal singles out certain directions of its total magnetization, in the case of pyrrhotite  $0^\circ$ ,  $60^\circ$ ,  $120^\circ$ ,  $180^\circ$ ,  $240^\circ$  and  $300^\circ$ , corresponding to its axes of symmetry. Further, since the elementary magnets constitute its total magnetization, exactly these directions of the elementary magnets also are distinctive (note that Lenz is not saying that the elementary magnets can *only* occupy positions that correspond to the symmetry of the crystal). All of these orientations of the elementary magnets are equivalent, and since they cannot rotate freely, they must have the ability to turn over from one position to the next. Lenz did not comment on how rapidly these turnovers occur, but Ising, in summarizing Lenz’s theory four years later in his thesis, wrote that they occur instantaneously.<sup>33</sup>

This turnover ability is the new assumption of Lenz’s theory. Brush (1967) asserted that its physical basis was the old quantum theory developed mainly by Niels Bohr and Sommerfeld. I find it difficult to see, however, where the old quantum theory enters into Lenz’s argument, because Lenz does not refer to it in describing the rotatability of the atoms in the crystals in question. Instead, his argument rested simply on Weiss’s observations concerning their symmetry.

<sup>30</sup> Lenz (1920), p. 614.

<sup>31</sup> Weiss (1905).

<sup>32</sup> Lenz (1920), p. 614.

<sup>33</sup> Ising (1924), p. 2.

To explain the Curie law, Lenz considered a bar magnet that was allowed to perform turnovers and was implicitly confined to a plane whose deflection from its equilibrium position was given by the angle  $\alpha$ . Two directions were singled out because:

In a quantum treatment certain angles  $\alpha$  will be distinguished, among them in any case  $\alpha = 0$  and  $\alpha = \pi$ . If the potential energy  $W$  has large values in the intermediate positions, as one must assume taking account of the crystal, then these positions will be very seldom occupied, Umklapp processes [turnovers<sup>34</sup>] will therefore occur very rarely, and the magnet will find itself almost exclusively in the two distinguished positions, and indeed on the average in each one equally long.<sup>35</sup>

The basis of Lenz’s “quantum treatment” probably was the idea of space quantization as set forth in 1916 by his former supervisor and later colleague in Munich, Arnold Sommerfeld, according to which the vector normal to the orbit of an electron, which is proportional to its magnetic moment, is allowed to point only in certain discrete directions relatively to an external magnetic field.<sup>36</sup> Space quantization, however, was first confirmed experimentally by Stern and Walter Gerlach in 1921, that is, after Lenz published his paper, so it seems likely that he quickly accepted Sommerfeld’s idea. This is corroborated in a letter that Ising wrote to Stephen G. Brush:

At the time I wrote my doctor thesis [under Lenz] Stern and Gerlach were working in the same institute on their famous experiment on space quantization. The ideas we had at that time were that atoms or molecules of magnets had magnetic dipoles and that these dipoles had a limited number of orientations.<sup>37</sup>

In sum, Lenz justified his crucial assumption that the elementary magnets will turn over between two positions first by arguing that their free rotatability was incompatible with Born’s theory of crystal structure; then by assuming that they can perform turnovers as suggested by experiments on ferromagnetic materials; and finally by concluding that in a quantum-theoretical treatment they would by and large occupy two distinct positions. His justification for his assumptions thus was based on a mixture of experimental and theoretical considerations, and the carefulness of his chain of argument indicates that he considered his assumption not just tentative, but as essentially correct.

Lenz pointed out that in his theory the time average of the magnetic moment vanishes when an external magnetic field is present and the directions corresponding to the angles  $\alpha$  and  $\pi - \alpha$  are assumed equally often. If, however, an external magnetic field of strength  $H$  is applied along the direction corresponding to the angle  $\alpha$ , say, then the difference in potential energy corresponding to the two directions is given by  $\mu H$  where  $\mu$  is the magnetic moment of the bar magnet. In that case, Lenz used Boltzmann’s principle to show that the average magnetic moment  $\bar{\mu}$  of the bar magnet is no longer zero but is given by:

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<sup>34</sup> I prefer the word “turnovers” because “Umklapp processes” have another meaning in solid-state physics.

<sup>35</sup> Lenz (1920), p. 614; translation follows Brush (1967).

<sup>36</sup> Mehra and Rechenberg (1982a), p. 435.

<sup>37</sup> Quoted in Brush (1967), p. 886; Ising’s letter is in English.

$$\bar{\mu} = \frac{\mu(e^a - e^{-a})}{e^a + e^{-a}}, \quad (12)$$

where  $a = \frac{\mu H}{kT}$ .

For sufficiently small  $a$ , this becomes  $\bar{\mu} = \frac{\mu^2 H}{kT}$ , that is, the Curie law.

So far, the assumption has been that the elementary magnets do not interact, which is presumably the case for paramagnetic materials, but is not the case for ferromagnetic materials. Lenz did not specify a definite interaction in the latter case but concluded that:

If one assumes that in the ferromagnetic bodies the potential energy of an atom (elementary magnet) with respect to its neighbors is different in the null position and in the  $\pi$  position, then there arises a natural directedness of the atom corresponding to the crystal state, and hence a spontaneous magnetization. The magnetic properties of ferromagnetics would then be explained in terms of nonmagnetic forces, in agreement with the viewpoint of Weiss . . . .<sup>38</sup>

Lenz, however, did not provide any calculations to support his optimism that this assumption would be sufficient to explain ferromagnetism.

### Ising's thesis and paper

After Lenz moved from Rostock to Hamburg,<sup>39</sup> he assigned the calculational tasks on his model to his student Ising, who wrote up his results in his thesis of 1924<sup>40</sup> and in a paper of 1925. Since there is no essential difference between the results that Ising presented in his thesis and in his paper, and since the former is more elaborate than the latter, I will focus on the former and only occasionally digress to the latter. There is a significant discrepancy between the two regarding the interpretation of his results, however, to which I will return later.

### *Ising's assumption*

Ising adopted Lenz's assumptions, but in addition employed a specific form of the interaction between the elementary magnets. At the same time, since Lenz was Ising's thesis advisor, one has to be careful to not draw rigid conclusions about the originator of the ideas in Ising's thesis simply because Ising published them. Indeed, as Ising wrote to S. Kobe: "I like to point out that the model really should be called [the] Lenz-Ising model. My supervisor, Dr. Wilhelm Lenz, had the idea and proposed that I make a mathematical workout as my dissertation. . . ."<sup>41</sup> As we will see later, the particular form

<sup>38</sup> Lenz (1920), p. 615; translated by Brush (1967), pp. 884–885.

<sup>39</sup> Brush (1967), p. 885.

<sup>40</sup> According to the title page, "Dissertation to obtain the doctorate [*Doktorwürde*] of the mathematical-scientific faculty of the University of Hamburg."

<sup>41</sup> Kobe (2000), p. 653; Ising's letter is in German.

of the interaction that Ising introduced was one of the main targets of criticism by his contemporaries.

With Lenz, Ising endorsed Weiss's view that the physical origin of the interaction between the elementary magnets was nonmagnetic in nature, since it was well known by that time that magnetic forces are too weak to give the right order of magnitude for the Curie temperature. Thus, the German physicist Walter Schottky (1886–1976) concluded in 1922, as Ising noted below, that the interaction was electrostatic in nature, because he was able to obtain the right order of magnitude for the Curie point by estimating the electrostatic energy in crystals. Ising, however, did not take a stand on the physical origin of the interaction:

In addition to an applied external magnetic field, the elements should also be affected by the forces that they mutually perform on each other. These forces may be of an electric nature [he cites here Schottky (1922)], but we cannot make a closer description of them; however, we assume that they decay rapidly with distance, so that we, in general, to a first approximation, only have to take the influence on neighboring elements into account. The latter assumption is somewhat in contrast with the hypothesis of a molecular field, which Weiss . . . has shown is not of a magnetic nature. We assume that of all the possible positions that the neighboring atoms can assume in relation to each other, the one that requires the minimum energy is when they are both acting in the same direction.<sup>42</sup>

Ising's last assumption of a minimum energy is crucial to explain the ordering of the elementary magnets in ferromagnetic materials. It is not clear whether Ising did not justify this assumption and that of the short range of the interaction because he considered them to be obviously correct, or because he was unable to give an argument for their correctness, even though he realized that both were necessary to explain ferromagnetism, in which case he may have considered them as working hypotheses. Thus, it is difficult to judge the extent of Ising's belief in the correctness of these assumptions.

Nonetheless, since Ising's introduction of them is crucial, I will try to uncover their origins. His first assumption of the short range of the interaction seems to have been inspired by Weiss's and Schottky's work, while his assumption of a minimum energy is more difficult to deal with, but also may have been inspired by Schottky's paper. Thus, Schottky had considered atoms placed horizontally in a plane with the magnetic moment of each atom arising from the revolution of its electrons, so that depending upon their direction of revolution the magnetic moment of each atom will point either up or down. He then argued that the electrostatic-potential energy between two neighboring atoms is a maximum when their electrons revolve in the same direction, so that it is smaller when the magnetic moments of the two atoms are parallel. This is in contrast to a situation in which the magnetic moments of the two atoms behave as macroscopic magnets, where the potential energy between them is larger for the parallel case than for the antiparallel case. Schottky, as noted above, was able to obtain the right order of magnitude for the Curie temperature from these considerations, and his idea of a minimum potential energy appealed to some of his contemporaries<sup>43</sup> and may have inspired Ising. Arguing against this suggestion, however, is that Schottky and Ising had different views on the

<sup>42</sup> Ising (1924), p. 4.

<sup>43</sup> Herzfeld (1925), p. 832.

orientation of the elementary magnets: Schottky took them to be pointing perpendicular to the plane in which they lay, while Ising always depicted them as pointing in this plane, at least in the case of a linear chain of them, which was his main object of study. Thus, if the chain extends horizontally, it consists of elementary magnets pointing left or right,  $\leftarrow$  and  $\rightarrow$ , respectively (and thus not the way the Lenz-Ising model is usually presented in modern textbooks). I conclude that because Schottky's argument does not apply to Ising's linear chain, it very likely did not stimulate Ising's conception of it. Another possibility here is connected to Ising's perception of the orientation of the elementary magnets. The configuration with the smallest *magnetic* energy is obtained when they point in the same direction (for instance  $\leftarrow\leftarrow$ ) instead of the opposite direction (for instance  $\leftarrow\rightarrow$ ). Since there seemed to be no reason to prefer the perpendicular orientation that Schottky proposed, Ising could choose the ones he did in a natural way and obtain the minimal potential energy, which is crucial for his explanation of ferromagnetism. A solid theoretical foundation for his choice was given only after the creation of the new quantum mechanics.

#### *Ising's linear chain*

Ising described his goal in introducing his concept of the linear chain as follows:

We now begin our task proper, the examination of the question whether ferromagnetism is explainable through the assumptions made. First, we carry this task out through a model as simple as possible; indeed through a linear magnet whose elements can assume only two positions. We shall find all essential results already present here.<sup>44</sup>

Ising then examined in detail and extended his concept of a linear chain of elementary magnets. Specifically, his linear chain consists of  $n$  elementary magnets placed equidistantly along a line, each of which has a magnetic dipole moment of magnitude  $m$  that is restricted to point in either of only two directions along it, so that two neighboring ones can assume only the following four configurations:  $\rightarrow\rightarrow$   $\leftarrow\leftarrow$   $\rightarrow\leftarrow$   $\leftarrow\rightarrow$ . It costs an inner energy  $\varepsilon$  to go from a configuration in which two neighboring elements have the same sign (the first two configurations) to one in which one of the elements is turned over by  $180^\circ$  (the second two configurations).

Ising evaluated the partition function  $Z$  for the linear chain when exposed to an external magnetic field of strength  $\mathfrak{H}$  by counting the total number of possible configurations and then, with the help of Eq. (5), he derived the following expression for the magnetization

$$\mathfrak{J} = mn \frac{\mathfrak{S} \sin \alpha}{\sqrt{\mathfrak{S} \sin^2 \alpha + e^{\frac{2\varepsilon}{kT}}}}, \quad (14)$$

where  $\alpha = \frac{m\mathfrak{H}}{kT}$ . Trigonometric functions written in fraktur are an old German notation for the corresponding hyperbolic functions.<sup>45</sup>

<sup>44</sup> Ising (1924), p. 5.

<sup>45</sup> See, for example, Courant (1930), p. 149.

Ising obtained the Curie law from Eq. (14) in the paramagnetic case, where  $\varepsilon/kT = 0$ , that is, when there is no interaction among the elementary magnets. He also showed that Eq. (14) implies that for the ferromagnetic case, if  $\mathfrak{H} \rightarrow 0$ , then  $\mathfrak{J} \rightarrow 0$ , that is, if the external magnetic field vanishes, the magnetization vanishes as well, so that the linear chain does not exhibit spontaneous magnetization. That to Ising was an "unwanted" result,<sup>46</sup> but it did not knock him out:

Under the assumptions made in the beginning and by means of the models considered previously [his linear chain and another model, irrelevant to my discussion], we succeeded only in explaining paramagnetism, and it is possible that perhaps only too crude an idealization does not let a ferromagnetic relation appear. It is imaginable that a spatial model, in which all elements that in some way are neighbors affect each other, brings with it the necessary stability to prevent the magnetization intensity to vanish with  $\mathfrak{H}$ . However, in that case the calculations do not seem to be feasible; at any rate, so far it has not been possible to sort and count the appropriate arrangement possibilities. To get a general overview of the situation, we shall make the following three considerations, in which we omit some of the previous simplifying assumptions.<sup>47</sup>

Ising's basis for his three considerations was three "complicated cases," which were generalizations of his linear-chain model. From my point of view, the most important one is the so-called spatial model, which is related to, but not identical with what today is termed the three-dimensional model, as I will discuss below. First, however, I will discuss Ising's other two generalizations because they provide further insight into his conception of his original model.<sup>48</sup>

In his first generalization, Ising took more positions of the elementary magnets into account. He allowed for so-called cross-positions in which each element can be oriented in  $r + 2$  directions, the usual two directions along the extension of the chain and another  $r$  directions perpendicular to it. Recall that Lenz, based on Weiss's result that the total magnetic moment is confined to the magnetic plane, assumed that the elementary magnets are situated only in this plane. Ising accepted Lenz's assumption of only two directions of the elementary magnets in his initial linear-chain model, but pictured the  $r$  cross-positions to be in the magnetic plane and the two original directions to be *perpendicular* to it. Thus, Ising's new assumption seems to contradict Lenz's assumption that the elementary magnets live in the magnetic plane. Ising did not discuss this contradiction, which seems hard to escape within the framework of his new model, either in his thesis or in his paper.

Ising's first generalization, nonetheless, sheds some light on his method of modeling, most notably on how physical phenomena restrict the model. The only restriction that Ising placed at first on the values of  $r$  was that they be even numbers, since for every allowed orientation of the elementary magnets, the opposite orientation is also

<sup>46</sup> Ising (1924), p. 15.

<sup>47</sup> *Ibid.*, pp. 24–25.

<sup>48</sup> In my presentation of Ising's generalizations, I have interchanged his second and third generalizations.



allowed. When Ising interpreted the elementary magnets as belonging to a particular solid, however, he imposed another restriction:

If we think of the sixfold axes of pyrrhotite as the longitudinal direction, then  $r = 6$ ; in contrast, we have to put  $r = 4$  for magnetite, corresponding to the fourfold symmetry of the axes. The  $r$  cross-positions all have equal roles.<sup>49</sup>

This is a physical and not a mathematical restriction on  $r$  because he carried out his calculations under the assumption that  $r$  is an arbitrary even number. Thus, it is not quite clear how realistic he considered this model to be, but because he restricted  $r$  to values that are compatible only with real magnetic materials, this suggests that he did not regard it just as a “toy model,” but instead regarded it to some extent as a realistic one.

Ising provided no arguments for the different energy costs associated with some of the arrangements of neighboring elements, but not to others that could be considered as equally important,<sup>50</sup> and he offered no clear physical basis for his choices. He did carry out some calculations of the general values of these energy costs, but only examined a special case in detail<sup>51</sup> for which he arrived at the same disappointing conclusion that he had come to for the case without cross-positions, namely, that it still did not yield any spontaneous magnetization.

Ising’s second generalization involved a linear chain with interactions between next-nearest-neighboring elementary magnets as well as between nearest-neighboring ones. He distinguished between the energy cost of the turnover of an elementary magnet in these two cases, but he made no assumption regarding the relationship between the two energy costs. He performed calculations similar to the ones in his first generalization and concluded as before, that the magnetic moment vanishes as the external magnetic field vanishes. Although he did not motivate his second generalization, it seems likely that he wanted to examine the range of the interaction by considering next-nearest neighboring elementary magnets as well as nearest-neighboring ones.

#### *Ising’s spatial model*

In his third and last generalization, Ising first examined interactions between elements in two linear chains and then in several linear chains. His double-chain model, however, does not shed new light on his methods of modelling, so I turn immediately to his several-chain model. Given, then,  $n_1$  parallel linear chains, he obtained what he called a spatial model (*räumlichen Modell*)<sup>52</sup> in which the magnetic moment of each

<sup>49</sup> Ising (1924), p. 25.

<sup>50</sup> Ising did not associate an energy cost with the arrangement of two cross-positioned elements.

<sup>51</sup> In this case, it costs the same energy for a positive as for a negative element to be a neighbor of a cross-positioned element.

<sup>52</sup> Since Ising’s paper is clearer than his thesis on this point, I shall follow the description in his paper here.

elementary magnet in one chain can assume two directions with respect to the one in the chain above or below it:

If similar poles of neighboring elements of the same chain collide at an inner position, then the crystal possesses the energy  $\varepsilon$  as before. In addition, it contains the energy  $\bar{\varepsilon}$  whenever two elements, one directly underneath the other, are directed oppositely.<sup>53</sup>

Ising’s model here must be seen as three-dimensional rather than two-dimensional, because he used the word “three-dimensional” in the abstract of his paper and in the paper itself where he termed his model spatial (*räumlichen*), whereas he had termed his earlier model planar (*flächenhaften*). Ising did not explain how the above arrangement of the chains constitutes a three-dimensional crystal, but his use of the word “layer” in relation to their cross section may suggest a regular organization of the elements so that their cross section looks like a two-dimensional square lattice with  $n_1$  points. From a mathematical point of view, however, the exact arrangement of the chains did not play an important role, because he further assumed that the energy  $\bar{\varepsilon}$  is so large that all  $n_1$  elements in a vertical layer point in the same direction, which means that a vertical layer can be treated as a single composite unit pointing in one direction and having a total magnetic moment  $n_1 m$ . In the limit of large  $\bar{\varepsilon}$ , each unit interacts with each other one in the same way as the elements in the original linear chain, but the interaction energy between oppositely oriented layers is  $n_1 \varepsilon$  instead of  $\varepsilon$ . With these substitutions into Eq. (14), Ising found that the magnetization is given by

$$\mathfrak{J} = mn_1 n \frac{\mathfrak{S} \sin(n_1 \alpha)}{\sqrt{\mathfrak{S} \sin^2(n_1 \alpha) + e^{n_1 \frac{2\bar{\varepsilon}}{kT}}}}. \quad (15)$$

It follows that there also is no spontaneous magnetization in Ising’s spatial model.

To a modern reader, because Ising reached this conclusion by considering his spatial model in the limit of large  $\bar{\varepsilon}$ , he destroyed any chance of reaching any conclusion about what we today would call the three-dimensional model. Ising himself, however, seemed to think that his conclusion could be extended to the “modern” three-dimensional model, since in the abstract of his paper he wrote:

It will be shown that such a model [the linear chain] does not have any ferromagnetic properties and that this statement also includes the three-dimensional model.<sup>54</sup>

Indeed, since Ising gave no indication that he restricted the class of spatial models to the class to which this general result applies, where his only assumptions were that of nearest-neighbor interactions and that of only a few orientations of the elementary magnets, he must have included in this class of spatial models the one that we today

<sup>53</sup> Ising (1925) pp. 257–258. My translation of Ising’s paper has been assisted by the translation by Jane Ising and Tom Cummings that can be found at [http://www.fh-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi\\_fm00.html](http://www.fh-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi_fm00.html).

<sup>54</sup> Ising (1925), p. 253.

would call the three-dimensional Ising model. In his thesis, however, Ising refrained from drawing that conclusion:

So, if we do not assume, as P. Weiss did, that also quite distant elements exert an influence on each other – and this seems to us not to be allowed under any circumstances – we do not succeed in explaining ferromagnetism from our assumptions. It is to be expected that this assertion also holds true for a spatial model in which only elements in the nearby environment interact with each other.<sup>55</sup>

Ising thus changed his mind on this point after writing his thesis and before publishing his paper. The reason seems to be, as he argued in his paper, that this particular spatial model, in which the elements can assume two directions, is more likely to exhibit ferromagnetism than a general spatial model in which cross-positions are allowed:

[The] positions of the moment perpendicular to the chain would demand too much energy to be realized. This assumption can be only favorable for the magnetization intensity along the direction of the chain which we consider.<sup>56</sup>

Ising inserted a footnote here referring to Weiss's results on pyrrhotite, probably meaning Weiss's observation that pyrrhotite cannot become magnetized in every direction but only in its so-called magnetic plane, which Weiss took to consist of rows of elementary magnets that can interact with each other only if they are in the same row. Since, however, the elementary magnets can rotate freely in the magnetic plane, they tend to become aligned along the direction of the row in the absence of an external magnetic field, but along its direction when one is present.<sup>57</sup> Ising thus concluded in his paper that:

Even though we here must expect a more favorable result than in a general spatial model, we recognize here, too, the vanishing of  $\mathfrak{J}$  with  $\mathfrak{H}$ .

So, in the model chosen here, whose essential trait is the restriction of the interaction between neighboring elements, ferromagnetism does not appear.<sup>58</sup>

In sum, Ising in his thesis opened up two possibilities for why the two basic assumptions of all his models – that the interaction between two elementary magnets is of short range and that the interaction energy is minimal when they act in the same direction – were incapable of explaining ferromagnetism.<sup>59</sup> First, either or both of these assumptions was not adequate (*zutreffend*). Second, contrary to Weiss's basic assumption and that of his successors, including Ising, thermal equilibrium did not apply to ferromagnetism, in which case Boltzmann's statistical theory could not be employed in explaining it. This possibility, according to Ising, was credible because of the phenomenon of spontaneous magnetization, that is, "the fact that a body once magnetized does not by itself change polarity, even though certainly no direction is energetically distinguished from its

<sup>55</sup> Ising (1924), p. 49.

<sup>56</sup> Ising (1925), p. 257.

<sup>57</sup> This history is discussed in Keith and Quedec (1992), p. 374.

<sup>58</sup> Ising (1925), p. 258.

<sup>59</sup> Ising (1925) does not discuss this issue.

opposite one.”<sup>60</sup> Ising did not elaborate on this point, but he could have meant that it “conflicts with Boltzmann’s theory, which implies that in the absence of an external magnetic field the polarity of a ferromagnet should point in each direction in an equal amount of time instead of always in the same direction. Ising did not settle on which of these two possibilities was more likely to explain why his models were not able to explain ferromagnetism, but they do reveal his uncertainty about its fundamental assumptions.

### Contemporary reactions to the Lenz-Ising model

Ising’s negative conclusion about the ferromagnetic behavior of the Lenz-Ising model might suggest that his contemporaries neglected it, especially because the creation of the new quantum mechanics in 1925–1926 had a dramatic impact on the theory of solids in general and on theories and models of magnetism in particular.<sup>61</sup> Thus, Samuel A. Goudsmit and George E. Uhlenbeck’s introduction of the concept of electron spin had clear implications for theories of magnetism, since it soon was realized that the ferromagnetic properties of matter were associated with the intrinsic spin angular momentum of the electron and not with its orbital angular momentum.<sup>62</sup> New fundamental theories of ferromagnetism soon appeared that might well have rendered the Lenz-Ising model obsolete shortly after it was proposed. In fact, however, it was not neglected. Why?

To attempt to answer this question, we must examine the reception of Ising’s work despite the sparsity of documentary evidence bearing on it. One document, however, consists of comments that Ising made in a letter to Stephen G. Brush concerning Ising’s “unwanted” conclusion that the linear chain results in no spontaneous magnetization:

I discussed the result of my paper widely with Professor Lenz and with Dr. Wolfgang Pauli, who at that time was teaching in Hamburg. There was some disappointment that the linear model did not show the expected ferromagnetic properties.<sup>63</sup>

Brush (1967) and Hoddeson, Schubert, Heims, and Baym (1992) convey the impression that by and large the Lenz-Ising model was not discussed by physicists before 1936, when Rudolf Peierls proved that the two-dimensional model in fact does display spontaneous magnetization at low temperatures. One main source for this impression is another passage in Ising’s letter above to Brush, where Ising (who had left physical research after finishing his degree in 1925) states that he was aware of only one contemporary citation to his work, namely, by Werner Heisenberg in his paper of 1928 in which he introduced his theory of ferromagnetism.<sup>64</sup> Incidentally, Ising used the term “contemporary” in quite a narrow sense, since he did not include under it a paper by Lothar Nordheim of 1934, which he also pointed out to Brush.

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<sup>60</sup> Ising (1924), p. 49.

<sup>61</sup> Hoddeson, Baym, and Eckert (1992), pp. 89, 123.

<sup>62</sup> Keith and Quedec (1992), p. 406.

<sup>63</sup> Brush (1967), p. 886.

<sup>64</sup> Heisenberg (1928a).

Nonetheless, Ising and others have exaggerated the neglect of the Lenz-Ising model. Although it is true that it was not cited in a host of publications on ferromagnetism in the 1920s and early 1930s, including, for instance, Edmund C. Stoner's two influential monographs on magnetism,<sup>65</sup> Heisenberg was not the only physicist to cite it.<sup>66</sup> Karl F. Herzfeld, in fact, cited Ising's paper already in 1925,<sup>67</sup> and both Wolfgang Pauli and John H. Van Vleck discussed Ising's results as well, Pauli in his paper given at the sixth Solvay Congress in October 1930,<sup>68</sup> which was devoted to magnetism and which was attended by most of the leading researchers in the field, and Van Vleck in his widely used textbook on magnetism.<sup>69</sup> Thus, although the number of contemporary citations to the Lenz-Ising model was not large, they included ones by the leading authorities in the field who exerted enormous influence on the subsequent theories of ferromagnetism.<sup>70</sup> Moreover, Ising's results and the Lenz-Ising model evidently were discussed personally among physicists in the late 1920s and early 1930s: Heisenberg referred to Ising's conclusions in a letter to Pauli in 1928,<sup>71</sup> and Peierls wrote in 1936 that Ising's results have "led to a good deal of controversy,"<sup>72</sup> a view he repeated in an interview in 1981.<sup>73</sup> Likewise, Hans A. Bethe stated in an interview in 1981 that the model "was discussed very much" in the early 1930s.<sup>74</sup> In sum, the Lenz-Ising model certainly was not neglected by physicists in the 1920s and early 1930s.

Ising's contemporaries generally seem to have accepted his result for the linear chain, but they rarely cited his negative conclusion for his three-dimensional model.<sup>75</sup> Herzfeld, for instance, did not mention it in 1925 when he stressed the importance of checking whether Ising's result for the linear chain also holds for his three-dimensional model.<sup>76</sup> At the same time, some physicists considered Ising's conclusion to be valid, while others did not. Thus, Peierls wrote in 1936 that "the opinion has often been expressed"<sup>77</sup> that the results for the three-dimensional case will be similar to those of the one-dimensional case, and in his autobiography of 1985<sup>78</sup> he recalled that he was so provoked by a mathematician who asserted the correctness of this conjecture in a talk, without offering proof, that he went home determined to prove the mathematician wrong.<sup>79</sup> Heisenberg

<sup>65</sup> Stoner (1926) and Stoner (1934).

<sup>66</sup> Heisenberg (1928b) cites this paper as well.

<sup>67</sup> I am grateful to Helge Kragh for bringing this important paper to my attention.

<sup>68</sup> Pauli (1932).

<sup>69</sup> Van Vleck (1932).

<sup>70</sup> Hoddeson, Baym, and Eckert (1992), pp. 123–124, 135; Keith and Quédec (1992), pp. 407–415.

<sup>71</sup> This letter can be found in Hermann, von Meyenn, and Weisskopf (1979), p. 467.

<sup>72</sup> Peierls (1936b), p. 478.

<sup>73</sup> Peierls interview with Hoddeson (1981), pp. 20–21.

<sup>74</sup> Bethe interview with Hoddeson (1981), p. 9.

<sup>75</sup> In 1938 Lamek Hulthén repeated Ising's conclusion uncritically; see Hulthén (1938), pp. 2, 15.

<sup>76</sup> Herzfeld (1925), p. 832. A later example is the controversy referred to by Peierls, which concerned exactly this point.

<sup>77</sup> Peierls (1936b), p. 478.

<sup>78</sup> Peierls (1985).

<sup>79</sup> This anecdote is pointed out by Hughes (1999), p. 106.

and Pauli, by contrast, seem to have believed that some variant of the three-dimensional model would display ferromagnetism. Thus, in a letter to Pauli in 1928,<sup>80</sup> Heisenberg suggested that if Ising had assumed sufficiently many nearest neighbors, probably more than eight (a number that Heisenberg himself had found to be necessary for the appearance of ferromagnetism), Ising would have obtained ferromagnetism. In 1930, Pauli too conjectured that the three-dimensional Lenz-Ising model very likely would display spontaneous magnetization.<sup>81</sup>

### *Heisenberg's theory of ferromagnetism*

Heisenberg's new theory of ferromagnetism of 1928 had a lasting influence on physicists' perception of the realism of the Lenz-Ising model. His interest in magnetism was not motivated by magnetic phenomena *per se*, but by the light they might shed on fundamental issues in quantum theory, that is, on the statistics of many-electron systems and on symmetries of the wave function.<sup>82</sup> He began by echoing Ising's criticism that Weiss's theory was only formally satisfactory in that it was based on the assumption that every atom in a crystal lattice is influenced by an aligning force arising from the other atoms whose origin, however, is unknown. He argued that the two obvious candidates for its origin were inadequate: It could not arise from the magnetic interaction between the atoms, because it is an order of magnitude smaller than the experimentally known atomic field, nor could it arise from the Coulomb interaction, which should be proportional to the square of the cosine of the angle between any two atoms, contrary to Weiss's assumptions. In proposing another candidate, he quoted Ising's result:

Other difficulties are discussed in detail by Lenz, and Ising succeeded in showing that also the assumption of aligning sufficiently great forces between each of two neighboring atoms of a chain is not sufficient to create ferromagnetism.<sup>83</sup>

Heisenberg's fundamental idea was that the angular deficiency of the Coulomb interaction can be remedied by combining the Coulomb interaction with Pauli's exclusion principle, which, more generally, also will be sufficient to reproduce the results of Weiss's theory.<sup>84</sup> To prove this, Heisenberg used the Coulomb exchange interaction, which he had introduced two years earlier to investigate the properties of helium, and which cannot be described in simple, intuitive language;<sup>85</sup> it leads to an interaction energy between pairs of electrons given by the so-called exchange integral. The case of helium with its two electrons seemed relevant to ferromagnetism, because of the strong spin-dependent

<sup>80</sup> Heisenberg to Pauli, July 31, 1928; reproduced in Hermann, von Meyenn and Weisskopf (1979), p. 467.

<sup>81</sup> Pauli (1932), p. 210. The publication of the proceedings was underway two years.

<sup>82</sup> Hoddeson, Baym, and Eckert (1992), p. 129.

<sup>83</sup> Heisenberg (1928a), p. 619; translated in Kobe (2000), p. 652. Brush (1967) gives a slightly different translation.

<sup>84</sup> Hoddeson, Baym, and Eckert (1992), p. 134.

<sup>85</sup> Van Vleck (1945), p. 30.

interaction energy between them. In 1929 P.A.M. Dirac derived<sup>86</sup> an explicit expression for the Hamiltonian

$$H = H_I + \sum_{i < k} H_{ik} \frac{1}{2} [1 + (\sigma_i, \sigma_k)], \quad (16)$$

where the sum is taken over the indices of the electrons,  $H_I$  and  $H_{ik}$  are terms independent of the spin  $\sigma$  of the electrons, and  $(\sigma_i, \sigma_k) = \sigma_{xi}\sigma_{xk} + \sigma_{yi}\sigma_{yk} + \sigma_{zi}\sigma_{zk}$ . This Hamiltonian, which was seen as characteristic of Heisenberg's theory, is sometimes called the Heisenberg-Dirac Hamiltonian. In any case, Heisenberg was able to derive Weiss's equation (Eq. (10) with  $H$  replaced by  $H_{total}$  of Eq. (11)) under the assumption that only nearest-neighbor interactions are nonnegligible, that the exchange integrals are the same for all electron pairs, and that the exchange energies have a Gaussian distribution.<sup>87</sup> He showed in this way that he could explain Weiss's molecular field in terms of the quantum-mechanical spin interaction. His contemporaries immediately accepted the exchange interaction as the correct mechanism behind ferromagnetism.<sup>88</sup> Nonetheless, they regarded his theory as only a step in the right direction, not as a final theory, and Heisenberg himself acknowledged some of its problems, including the arbitrariness of the Gaussian distribution.<sup>89</sup> Moreover, some physicists attacked his assumption that all of the nearest neighbors have the same exchange integral.<sup>90</sup>

The above approach is usually called the Heisenberg *theory* of ferromagnetism, whereas the term Heisenberg *model* is used for the situation in which the exchange energy is negligible except for nearest-neighbor pairs of atoms and is the same for all such pairs. In the Heisenberg model, the total interaction energy is given by the so-called Heisenberg Hamiltonian

$$H_I = -2J \sum_{\text{neighbors}} \sigma_i \cdot \sigma_j, \quad (17)$$

where  $J$  is the exchange energy, which is the same for all neighboring pairs,  $\sigma_i$  and  $\sigma_j$  are the spins of the  $i$  and  $j$  electrons (which are represented by vectors), and the sum is taken over all nearest-neighbor pairs of atoms in the crystal lattice.

#### *The relationship between the Lenz-Ising model and Heisenberg's theory*

Lenz and Ising considered the elementary magnets in a crystal to arise from the magnetic moments of its atoms or molecules, while Heisenberg took them to arise from the spin angular momentum of the electrons in the atoms or molecules. Lenz and Ising

<sup>86</sup> Dirac (1929). In this paper, Dirac did not refer to Heisenberg.

<sup>87</sup> Hoddeson, Baym, and Eckert (1992), pp. 129–135.

<sup>88</sup> See, for example, the views expressed by Felix Bloch in Hoddeson, Baym, and Eckert (1992), p. 135; by John H. Van Vleck in Van Vleck (1932), p. 322; Edmund C. Stoner in Stoner (1934), p. 352, pp. 424–425; and Peierls in Peierls (1936b), p. 477.

<sup>89</sup> Hoddeson, Baym, and Eckert (1992), pp. 134–135.

<sup>90</sup> See, for instance, Van Vleck (1945), p. 32.

did not discuss the origin of the dipole moment of the atoms or molecules, but they no doubt believed that it arose from the revolution of their electrons about their nuclei.<sup>91</sup> Moreover, considering the skepticism with which several physicists greeted Goudsmit and Uhlenbeck’s concept of electron spin,<sup>92</sup> Lenz and Ising probably did not even consider electron spin as origin of the elementary magnets when they proposed their model.

That did not prevent Heisenberg from noting the similarity between the Lenz-Ising model and his own, for instance in a paper he wrote on the occasion of Arnold Sommerfeld’s 60th birthday in 1928:

[The] model grounded here [an extension of the Heisenberg model described above] actually shows great similarity with Ising’s model (only interaction between neighboring atoms) and differs essentially only through the value of  $z$  [the number of nearest neighbors in the lattice], i. e., through the number of neighbors that surround an atom.<sup>93</sup>

The first use of the term “Ising model” is usually ascribed to Peierls (1936b),<sup>94</sup> but we see here that Heisenberg used it eight years earlier, at least for the one-dimensional case.

Heisenberg, however, did not discuss Lenz and Ising’s assumptions from a more fundamental point of view, although his sparring partner Pauli did in the paper he gave at the sixth Solvay Congress in 1930, where he called the Lenz-Ising model “a semi-classical model”<sup>95</sup> and took its Hamiltonian (probably referring to the one-dimensional case) to be:

$$H = -A \sum_k (\sigma_k, \sigma_{k+1}), \quad (18)$$

where  $\sigma_k$  is the spin angular-momentum vector of the  $k$ th electron and the operator  $(\sigma_k, \sigma_{k+1})$  attains the value 1 if the spins of electrons  $k$  and  $k+1$  are parallel and  $-1$  if they are antiparallel. Thus, Pauli implicitly reinterpreted the Lenz-Ising model in terms of electron spins so that he (and others) took its basic constituents, the elementary magnets, to be different from Lenz and Ising’s and in that sense did not discuss the same model. Pauli was able to reinterpret the Lenz-Ising model in this way only because Lenz and Ising had focused on the general properties of the magnetic moment, not on the details of its origin.

Pauli now could view the Lenz-Ising model in light of the new quantum mechanics and Heisenberg’s theory of ferromagnetism, between which he saw a “narrow kinship”<sup>96</sup> as displayed by Dirac’s Hamiltonian Eq. (16) and Ising’s Hamiltonian Eq. (18). Pauli argued that since the electron spins  $\sigma_i$  in Eq. (16) are treated as operators in the new quantum mechanics, this also should be true for the magnetic moment  $m$  in the Lenz-

<sup>91</sup> This view is expressed by Schottky (1922) as cited in Ising (1925) and Ehrenfest (1921).

<sup>92</sup> Mehra and Rechenberg (1982b), pp. 199–204.

<sup>93</sup> Heisenberg (1928b), p. 122.

<sup>94</sup> See, for instance, Kobe (2000), p. 652.

<sup>95</sup> Pauli (1932), p. 209.

<sup>96</sup> *Ibid.*, p. 210.



Ising model. That, however, implied that the Lenz-Ising model was in conflict with the new quantum mechanics:

In Ising's calculus, developed from the point of view of the old quantum mechanics, the components of  $\sigma_i$  that are perpendicular to the field are considered to be zero, whereas in the new quantum theory these components do not commute with the components of the field.<sup>97</sup>

That conflict meant that to Pauli and others the Lenz-Ising model was fundamentally deficient.<sup>98</sup> As Hans A. Bethe remarked in 1981, endorsing Pauli's criticism of it:

Well, even if it was old, it was discussed very much at that time still [in the early 1930s]. But it clearly was not the right model, because the spin is a quantum object and not a classical object, so you couldn't just say up spin and down spin, but have to permit them to change direction.<sup>99</sup>

Others criticized the Lenz-Ising model because it conflicts with the Heisenberg model, which therefore must have been seen as the more realistic (or at least the more satisfactory) of the two. Specifically, the interaction assumed in the Lenz-Ising model was too simple when compared to that in the Heisenberg model. Thus, Van Vleck (1932) remarked in a footnote that Ising has assumed "arbitrarily" that the coupling between the elementary magnets was given by the first part of the scalar product in Eq. (16), rather than by the complete product as in the Heisenberg model. These objections to the Lenz-Ising model were so serious that it was dismissed as a realistic model of ferromagnetism in the early 1930s.

The advent of the new quantum mechanics may well have played other roles in the reception of the Lenz-Ising model among physicists as a model of ferromagnetism.<sup>100</sup> The Lenz-Ising model tacitly assumed that the interaction between the elementary magnets could be split into pairwise interactions, which may have prompted some uneasiness about its validity. In 1929 P.A.M. Dirac gave a quantum-theoretical justification for this assumption, although he did not refer explicitly to two-body interactions. Likewise, Ising's explicit assumption that the interaction is of short range was likewise put on a more secure theoretical footing in the new quantum mechanics. Finally, Heisenberg's model incorporated the restriction of the Lenz-Ising model to nearest-neighbor interactions. The Lenz-Ising model also fell short on the important issue of the details of the interaction and the noncommutivity of the spin with the field. Peierls thus concluded in

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<sup>97</sup> *Ibid.*

<sup>98</sup> Hoddeson, Schubert, Heims, and Baym (1992), p. 521, argue that the Lenz-Ising model was by and large ignored in relation to *critical phenomena* in the late 1920s and early 1930s, since the focus was on the details of the interaction, where the Lenz-Ising model fell short. It is not so clear what they are referring to by the term "critical phenomena" (they seem to use the term "critical phenomena" for what I called cooperative systems in introduction), because there was no general treatment on critical or cooperative phenomena in this period. However, if their argument is restricted to the area of ferromagnetism, it is correct, as shown by Pauli's treatment of the model.

<sup>99</sup> Bethe with Hoddeson (1981), p. 9.

<sup>100</sup> This interesting point was made to me by an anonymous reader to whom I am thankful for it.

1936 that, "The Lenz-Ising model is therefore now only of mathematical interest."<sup>101</sup> Why, then, did he as a physicist study it? He commented:

Since, however, the problem of Ising's model in more than one dimension led to a good deal of controversy and in particular since the opinion has often been expressed that the solution of the three-dimensional problem could be reduced to that of the linear model and would lead to similar results, it may be worth while to give its solution.<sup>102</sup>

In 1981 Peierls recalled a more substantial motivation for studying the Lenz-Ising model:

It is true that at that time [around 1936], Ising's paper was rather old, but interest in ferromagnetism had grown recently because with the advent of quantum theory. Heisenberg had shown the physical basis of ferromagnetism; [Felix] Bloch and Bethe had given approximations to the theoretical problem of ferromagnetism. And so, while all this was leading to rather complicated mathematical problems, one did look back to the very simple and attractive model of Ising.<sup>103</sup>

Bethe recalled yet another reason: He thought that the Lenz-Ising model might shed some light on the temperature dependence of ferromagnetism, but he published nothing on this problem.

After Peierls dismissed the Lenz-Ising model as a model of ferromagnetism in 1936, it was rarely discussed in that connection, and when it was mainly in a negative light. Thus, in a paper published in 1945 but based upon lectures he delivered in 1939,<sup>104</sup> Van Vleck (1945) viewed the Lenz-Ising model only as a simplification of Heisenberg's model with a truncated interaction and repeated his criticism of 1932, only more sharply:

In a certain sense the Lenz-Ising model is a purely mathematical fiction, as it neglects the interactions  $-2J(s_{x_i}s_{x_j} + s_{y_i}s_{y_j})$  between the components of spin perpendicular to the direction of the magnetic field, which are often important physically.<sup>105</sup>

He continued to carve up the Lenz-Ising model, stating that even if it could serve as the basis for rigorous calculations for three-dimensional lattices, "the result should not be identified too closely with the actual magnetic behavior of the material simply because of the inadequacy and arbitrariness of the model."<sup>106</sup> He saw its only role as providing mathematical insight into eigenvalue problems associated with magnetic materials, and thus into solutions of Heisenberg's model. It was not significant in its own right as a model of ferromagnetism.

<sup>101</sup> Peierls (1936b), p. 477.

<sup>102</sup> *Ibid.*, pp. 477–478.

<sup>103</sup> Peierls with Hoddson (1981), pp. 20–21.

<sup>104</sup> Although published in 1945, a footnote (p. 27) states it is based "to a considerable extent" on one of several lectures given in Paris in 1939. They were meant to be published in the *Annales de l'Institut Henri Poincaré*, but the publication was delayed by the German invasion of France, and they first appeared in Van Vleck (1947).

<sup>105</sup> Van Vleck (1945), p. 34.

<sup>106</sup> *Ibid.*, p. 34.

Van Vleck was a leading authority on magnetism, so it seems fair to conclude that most researchers in the field rejected the Lenz-Ising model as a model of ferromagnetism by 1945, and probably even earlier. Subsequently, it sometimes was referred to as a model of ferromagnetism, and to the extent that its realism was discussed, it was described as unrealistic.<sup>107</sup> A shift occurred, however, in the 1950s when it was used to model the magnetic properties of some pure rare-earth elements and good agreement was found with such real elements, because both have a strong anisotropic interaction; some differences, however, remained.<sup>108</sup>

I should note, at the same time, that there were at least two positive responses to the Lenz-Ising model in the field of ferromagnetism before 1945. Francis Bitter devoted ten pages to Ising's linear chain in his textbook of 1937 although he considered Heisenberg's model as more realistic. Still, Ising's result for the linear chain "has taken on a new importance,"<sup>109</sup> first, because materials that can be represented by it might be found in the future, and second, and more importantly, because Ising's result was a rigorous one, in contrast to Heisenberg's. Kramers and Wannier, however became the most prominent advocates of the Lenz-Ising model in the years 1936–1945, as I will discuss later. We will see that they were not very clear about its realism in relation to ferromagnetism, but they definitely considered its study as being worthwhile.

I have argued above that the problematic relationship between the Lenz-Ising model and the new quantum theory was largely responsible for its dismissal. Others, however, have claimed that the main reason for ignoring it as a model of ferromagnetism was Ising's negative conclusion for the three-dimensional case. Brush (1967) and Keith and Quedec (1992) have advanced this claim, which now seems to be widely accepted.<sup>110</sup> Two objections, however, can be raised against it. First, as I have shown, it is not entirely clear that Ising's contemporaries accepted his negative conclusion; indeed Heisenberg and Peierls did not, and others may have shared Peierls's opinion that spontaneous magnetization may appear in the two-dimensional and three-dimensional cases, even before Peierls proved that it did. Second, even if some physicists had accepted Ising's negative conclusion, they still may have accepted the Lenz-Ising model. Thus, Peierls's proof seems to have had no impact on his opinion of the realism of the Lenz-Ising model, since in the same paper he suggested that it was only of mathematical interest. Thus, it is hard to maintain that the question of whether or not it can display spontaneous magnetization was decisive for not accepting it as a reasonable representation of ferromagnetism.

### Peierls's proof

Ironically, despite Peierls's view that the Lenz-Ising model was only of mathematical interest, his paper of 1936, in which he proved that spontaneous magnetization appears in the two-dimensional and three-dimensional cases, was one of the most important

<sup>107</sup> See, for example, ter Haar and Martin (1950), p. 721; Newell and Montroll (1953), p. 353; or Yang (1952), p. 808.

<sup>108</sup> Wolf (2000), p. 794.

<sup>109</sup> Bitter (1937), p. 145.

<sup>110</sup> See, for instance, Hughes (1999), p. 104; and Mattis (1985), pp. 89–90.

ones in its early history. He showed that at sufficiently low temperatures the Lenz-Ising model in two dimensions does display ferromagnetism,<sup>111</sup> that is, the ratio  $M = \frac{n_+ - n_-}{n_+ + n_-}$  is nonzero, and from his proof he concluded that this is also true in three dimensions. His proof, which uses quite elementary techniques, goes like this: He placed boundaries midway between every pair of nearest magnets of opposite signs, thus separating areas of positive magnets from ones of negative magnets by connected boundaries, which are open if they begin and end at the edges of the crystal lattice and are closed if they do not. He then first made an upper estimate of the number of open boundaries and showed that for a sufficiently large array, the elementary magnets enclosed by them do not play an important role. Second, he estimated the number of closed boundaries and, knowing that a boundary of length  $L$  in lattice units corresponds to an energy  $UL$  (since each boundary element separates two magnets of opposite signs), he concluded that the number of magnets enclosed by closed boundaries decreases with decreasing temperature: When, say,  $4e^{U/kT} < 0.8$ , the number enclosed is smaller than  $1/4$ . Thus, for sufficiently low temperatures, less than half of the magnets are enclosed by open and closed boundaries and the ratio  $M/N$  is nonzero, that is, the system displays spontaneous magnetization.

### The transition to a model of cooperative phenomena

#### *Cooperative phenomena*

Since the Heisenberg model was considered as a much more realistic model of ferromagnetism than the Lenz-Ising model by the end of the 1920s, why was the Lenz-Ising model not simply forgotten in the 1930s and 1940s? Why was it studied then despite its apparent lack of realism as a model of ferromagnetism? The answer to these questions are closely linked to developments in the theories of alloys, adsorption, and cooperative or collective phenomena.<sup>112</sup>

Nix and Shockley (1938) and Brush (1967) have recounted these developments in the field of alloys. Thus, the Russian-German chemical physicist Gustav Tamman carried out experiments in 1919 that showed that an alloy of 50% copper and 50% gold forms an ordered array of atoms, superlattices, which X-ray experiments a few years later showed also exist in other alloys. Their characteristic feature is that the atoms of one of their components tend to be surrounded by the atoms of the other component, an example being the superposition of two cubic lattices, where the sites of one lattice are in the middle of the other one. At low temperatures, a superlattice is in an ordered state in which each site is occupied by an atom of the "right" kind, and when it is heated

<sup>111</sup> This proof was later considered to be incorrect by N.G. van Kampen, M.E. Fisher, and S. Sherman, because the summations were over all lengths of the boundaries, that is, including infinite, even for finite systems. R.B. Griffith was able to provide a rigorous proof along the same lines as Peierls; see Kobe (2000), p. 652.

<sup>112</sup> Some historians and philosophers, for instance, Liu (1999), discriminate between cooperative and collective phenomena, whereas others, for instance Hoddson, Baym, and Eckert (1992), do not. In the period that I consider, this type is called cooperative phenomena, and I shall stick to that term throughout.

thermal agitation enhances the amplitudes of vibrations of both atoms, and they can acquire sufficient energy to change sites. The two atoms then are in the “wrong” sites, which decreases the order of the superlattice.

Bragg and Williams (1934) developed a statistical-mechanical theory of this phenomenon based on the idea that the energy cost of moving an atom from a “right” to a “wrong” site is proportional to the degree of disorder previously present in the superlattice.<sup>113</sup> Bethe (1935) noted that their theory and Weiss’s theory of ferromagnetism share the assumption that the “force” trying to produce order at a given site in the lattice depends on the average order of the system; in effect, the two theories use similar mathematical methods. Bethe, however, stressed that in both theories the force ought to depend on the particular configuration of the atoms in the neighborhood of the site in question. Accordingly, he refined Bragg and Williams’s theory by assuming that only nearest-neighbor atoms interact, with energies of  $V_{ab}$ ,  $V_{aa}$ , and  $V_{bb}$  between an  $A$  and a  $B$  atom, two  $A$  atoms, and two  $B$  atoms, respectively. He pointed out that this “assumption is essentially the same as that which underlies the modern theory of ferromagnetism [Heisenberg’s theory],”<sup>114</sup> which therefore also should embody the notion of order:

[Experimentally] a sharp Curie point is found at which the “order,” i.e., the permanent moment, of the crystal as a whole disappears. Super-lattices should be similar, and one may even hope that it is simpler to treat since it involves no quantum mechanics but only classical statistics.<sup>115</sup>

To pursue this idea, Bethe introduced the important Bethe approximation (sometimes called the Bethe-Peierls approximation).<sup>116</sup>

In 1936 Ralph H. Fowler in Cambridge proposed a statistical theory of adsorption to account for experiments in which a stream of metal vapor was sent towards a glass surface and a critical temperature  $T_c$  was found that separates a low-temperature from a high-temperature regime in which the metal vapor can or cannot be deposited on the glass.<sup>117</sup> Fowler pointed out that although this phenomenon had been studied earlier by Irving Langmuir in 1916 and Yakov I. Frenkel in 1924, his model assumed that the metal vapor is in equilibrium with the glass surface, which consists of a regular array of  $N$  sites, each of which is a possible site for the adsorption of exactly one metal atom, that is, the film forms a monolayer below which no metal atoms can penetrate. The adsorption energy  $\chi_0$  for each adsorbed atom corresponds to the force exerted on it by the glass, and each pair of neighboring adsorbed atoms has an interaction energy  $V = -\chi_0/z$ . The problem is to determine the ratio  $M/N$ , where  $M$  is the total number of adsorbed atoms

<sup>113</sup> Gorsky had made a similar theory earlier, but without receiving the credit he deserved; see Domb (1996), p. 17.

<sup>114</sup> Bethe (1935), p. 552.

<sup>115</sup> *Ibid.*, pp. 552–553.

<sup>116</sup> Technically speaking, in this approximation the focus is on a certain site, called the central site or atom and its nearest neighbors, called the first shell. The nearest neighbors of the first shell (excluding the central site) are called the second shell. The effect of the second shell on the first shell is approximated by the same factor for all sites in the second shell, independent of their actual arrangement.

<sup>117</sup> Fowler (1936).

and  $N$  is the number of possible sites that can be occupied by an atom. Fowler (1936) applied the Bragg-Williams theory and Peierls (1936a) applied the Bethe approximation to this problem.

Physicists recognized that such phenomena had certain features in common, both from an experimental and from a theoretical point of view. As Peierls wrote in 1934:

For many, physically very diverse but formally analogous, phenomena it is found experimentally that a transition takes place from an ordered state to a state of disorder at a certain temperature. . . . Typical examples for this are the melting points of solids and the Curie point of ferromagnetism.<sup>118</sup>

According to Fowler the sharpness of transition points was an “ancient problem,”<sup>119</sup> but the recognition that physically diverse systems exhibit them experimentally was new. That also was true theoretically between various theories and models. As Brush (1967) pointed out, Fowler and his collaborators at Cambridge (including Peierls) seem to have been the first to recognize the analogy between a number of different problems;<sup>120</sup> they applied the idea of order-disorder in alloys and the Bragg-Williams theory to other cooperative phenomena, such as the rotation of molecules in solids and the adsorption of gases.

Fowler, in the second edition of his textbook on statistical mechanics of 1936, concluded that the essential general feature of a large class of phenomena, including the ones described above, is cooperation, and he thus termed them *cooperative* phenomena.<sup>121</sup> Such systems can be described only in terms of the joint action of the units constituting them, that is, the behavior cannot be captured by treating the units approximately as independent. Fowler focused on individual phenomena whose theories or models involve the cooperation of units and discussed these in great detail; he did not provide a general theory of cooperative phenomena – that was simply a convenient umbrella for phenomena that did not fit into other classifications, not a fundamental entity requiring explanation. He treated the theories or models of ferromagnetism and alloys, for example, as distinct even after their mathematical equivalence was known. Thus, for example, he formulated the Bethe theory specifically in terms of binary alloys and compared it to experimental data and thus focused specifically on such alloys and not on cooperative phenomena in general. Still, others suggested otherwise. For example, John G. Kirkwood, then at the University of Chicago and Cornell University, wrote:

<sup>118</sup> Peierls (1934), p. 137. This description was given at a conference on the theory of metals in Geneva in 1934.

<sup>119</sup> Fowler (1934), p. 74.

<sup>120</sup> Brush (1967) states that Fowler considered the Ising model, which is not quite correct. I will discuss this point below.

<sup>121</sup> Independently of Fowler, Fritz Zwicky of the California Institute of Technology developed an approach to cooperative phenomena that was more ambitious. Indeed, Zwicky (1933) coined the term “cooperative phenomena.” There is some overlap between the phenomena classified as cooperative in the two approaches, but it is far from complete. Since Fowler’s took root and are related to the development of the Lenz-Ising model, I restrict my treatment to his approach.

We believe that the theory may prove useful not only in the study of order and disorder in solids, but also in the treatment of cooperative phenomena in general.<sup>122</sup>

### *Cooperative phenomena and the Lenz-Ising model*

According to Brush (1967), Peierls (1936b) first recognized the *mathematical* similarity of the Lenz-Ising model to other theories of cooperative phenomena, writing that Bragg and Williams's and Bethe's theories of alloys, Fowler's theory of the libration-rotation transition point in solids, and some other theories as well, are all physically different but mathematically equivalent.<sup>123</sup> Peierls probably regarded them as physically different because they do not stem from the same physical mechanism or deal with the same physical objects or situations, but they are mathematically equivalent because they obey the same equations. Strictly speaking, however, Peierls only proved the mathematical equivalence of the theory of adsorption and of the Lenz-Ising model. He replaced the empty and occupied sites in the theory of adsorption by minus and plus signs for the elementary magnets and the quantity  $2M-N$  by the total magnetic moment and in this way was able to establish the mathematical equivalence between Fowler's theory of monolayer adsorption and the Lenz-Ising model, since the equations for both systems are identical. The results of one can thus be applied to the other; for instance, the adsorption transition point and the Curie ferromagnetic temperature are equal when the Bethe approximation is applied to both.

There were historical precedents for such mathematical analogues. For instance, in the nineteenth century, Pierre Simon Laplace (1749–1827) and Simon Denis Poisson (1781–1840) established the mathematical equivalence between Fourier's theory of heat flow and the theory of electromagnetic action, which allowed William Thomson (1824–1907) to transfer the mathematical results of the former theory to the less-developed latter theory.<sup>124</sup> More generally, several physicists in the nineteenth century recognized that the same partial-differential equations can be applied to physically different continuum systems: Such mathematically equivalent theories were common knowledge by the 1930s<sup>125</sup> and may have facilitated the acceptance of the Lenz-Ising model as an abstraction of more concrete physical systems.<sup>126</sup>

At the same time, because the different theories of alloys, adsorption, and ferromagnetism were not treated in common in the 1930s, this indicates that one should be cautious in using the term “Lenz-Ising model.” Today, it is associated mainly with its mathematical structure, more or less detached from any specific physical phenomenon like ferromagnetism. Peierls's recognition that the Lenz-Ising is mathematically equivalent to other theories of cooperative phenomena, however, did not prompt physicists to search for a unified structure of them in the 1930s and the early 1940s. The Lenz-Ising

<sup>122</sup> Kirkwood (1938), p. 70.

<sup>123</sup> Peierls (1936b).

<sup>124</sup> See, for example, Smith and Wise (1989), pp. 202–212; and Cat (2001), p. 419.

<sup>125</sup> Purrington (1997), p. 170. Whittaker and Watson (1927), pp. 386–387, mentioned six different branches of mathematical physics where Laplace's equation occurs.

<sup>126</sup> I am grateful to an anonymous reader for this point.

model then was always considered to be a model of ferromagnetism, and not one also of alloys, for instance, whose mathematically equivalent treatment was called the Bethe method applied to alloys. Thus, one has to distinguish carefully between the mathematically equivalent models of different physical phenomena in the 1930s and 1940s, which has not always been done.<sup>127</sup>

In contrast to the appellation Lenz-Ising *model*, treatments of the behavior of binary alloys and adsorption are all called *theories* by researchers in these fields. In view of the great similarity between the Lenz-Ising model and the theories of alloys and adsorption, however, we might ask whether the distinction between "model" and "theory" that was used in the 1930s and early 1940s reflects a fundamental distinction between these two concepts. I first note that the mathematical similarity of the theories of alloys and ferromagnetism was well known: Bethe (1935) noted the analogy between Bragg and Williams's theory of alloys and Weiss's theory of ferromagnetism, and the analogy between his own theory of alloys and the quantum theory of ferromagnetism. Furthermore, all three theories were viewed as drastically simplified representations of real materials. For instance, the interactions between atoms in the two theories of alloys and between spins in the Lenz-Ising model of ferromagnetism are both quite crude, and none are based on the new quantum theory, which was viewed as the correct fundamental theory for all of them. It therefore seems that the only essential difference between the treatments of ferromagnetism and of alloys that can justify different labels is that the Lenz-Ising model was known to be an approximation to the Heisenberg theory of ferromagnetism, whereas no analogous fundamental theory existed for alloys. Thus, the theories of alloys could be viewed as first steps towards such a fundamental theory of alloys, whereas that was impossible for the Lenz-Ising model in its relationship to a fundamental theory of ferromagnetism. Still, since the terms "theory" and "model" were used in different physical contexts, they need not have been used consistently between them.

In general, while physicists did not focus much on the Lenz-Ising model in the theory of ferromagnetism in the 1930s and early 1940s, they used its mathematical equivalent extensively in the theory of binary alloys during this period.<sup>128</sup> That, however, did not change their attitude towards it, so I will not pursue that development further here.

<sup>127</sup> For instance, Brush (1967), p. 887, wrote: "The concept of the 'Ising model' as a mathematical object existing independently of any particular physical approximation seems to have been developed by the Cambridge group led by R. H. Fowler in the 1930's." In the 1930s, Fowler discussed the Bethe theory of alloys and his own theory of adsorption, and even though they are mathematically equivalent to the Lenz-Ising model, Fowler made no reference to this model. From a historical point of view, it is therefore not correct to conclude that he discussed the Lenz-Ising model, but rather two of its mathematical equivalents.

<sup>128</sup> See, for example, Kirkwood (1938), pp. 70–75; Nix and Shockley (1938), pp. 2–30; Bethe and Kirkwood (1939), pp. 578–582; and Lassetre and Howe (1941), pp. 747–754.



### The Lenz-Ising model in the 1940s

In the early 1940s, the papers in which the Lenz-Ising model was discussed were not aimed at understanding particular physical systems but rather transition points and cooperative phenomena in general.

I will examine the quite different motivations of Elliott Montroll (1916–1983), Hendrik A. Kramers (1894–1952) and Gregory Wannier (1911–1983), and Lars Onsager (1903–1976) for studying the Lenz-Ising model. They all were part of the same network of researchers,<sup>129</sup> with the young Montroll being an important link in it. Thus, Wannier taught Montroll statistical mechanics as a graduate student in chemistry at the University of Pittsburgh,<sup>130</sup> but he then shifted to mathematics and received his Ph.D. degree with a thesis on the evaluation of integrals appearing in the theory of imperfect gases. He subsequently spent the academic year 1940–1941 as a postdoctoral fellow at Yale University with Onsager<sup>131</sup> where he told Onsager about his and Wannier's ideas on the Ising problem.<sup>132</sup>

#### Montroll

Montroll published a paper entitled “Statistical Mechanics of Nearest Neighbor Systems” in 1941, calling attention to a host of studies on such physical systems, which are characterized by an interaction between molecules of sufficiently short range to allow them to be modelled by taking into account only nearest-neighbor interactions. These studies dealt with several areas I discussed earlier, for instance, order-disorder phenomena in alloys and the Lenz-Ising model of ferromagnetism. He noted, however, “that no general mathematical technique for the handling of these problems (which are abstractly alike) has been developed.”<sup>133</sup>

Montroll then developed an elaborate “general theory,”<sup>134</sup> a general mathematical theory of nearest-neighbor systems, by reducing the partition function to equations of linear homogeneous operators. He applied his theory to the “two-dimensional ferromagnetic net,” that is, the two-dimensional Lenz-Ising model, but only “as a medium of demonstration,”<sup>135</sup> explicitly avoiding an interpretation of it. He had more substantial things to say, however, about phase transitions:

As one raises the temperature of a physical system (containing a large number of molecules) in a given state there often exist temperatures at which the system undergoes a radical change in state. For example, in a solid with a definite crystal structure the lattice

<sup>129</sup> Hoddeson, Schubert, Heims, and Baym (1992), p. 528.

<sup>130</sup> *Ibid.*, p. 529.

<sup>131</sup> Montroll also spent the academic year 1939–1940 at Columbia University with the chemical physicist Joseph E. Mayer (with whom he published a paper on imperfect gases in 1941) and the academic year 1941–1942 at Cornell University with John Kirkwood; see Weiss (1994), p. 365.

<sup>132</sup> Hoddeson, Schubert, Heims, and Baym (1992), p. 531; Onsager (1971), p. xxi.

<sup>133</sup> Montroll (1941), p. 706.

<sup>134</sup> *Ibid.*

<sup>135</sup> *Ibid.*, p. 713.

is sharply disrupted at a temperature called the melting point, and above this temperature the liquid state exists. There is a temperature at which a ferromagnetic material sharply loses its magnetic properties. Such changes in state are called phase changes or phase transitions. At the transition temperature both states are equally probable and can coexist at equilibrium in any proportion. . . .<sup>136</sup>

Montroll connected these qualitative properties of phase transitions to his mathematical description of nearest-neighbor systems by using Frobenius's theory of matrices, obtaining the important result that for a "sharp phase transition"<sup>137</sup> to occur in a square two-dimensional square lattice, the lattice has to extend infinitely far in both directions.

In sum, because Montroll's focus was on the mathematical exploitation of the similarities of nearest-neighbor systems, and because he considered these systems to be only "abstractly alike," his purpose should be seen as an attempt to establish a general mathematical theory of nearest-neighbor systems rather than as an attempt to provide a general physical theory of cooperative phenomena.

#### *Kramers and Wannier*

In their two-part paper on the "Statistics of the Two-Dimensional Ferromagnet" of 1941,<sup>138</sup> Kramers and Wannier were more interested than was Montroll in the physical aspects of the Lenz-Ising model. Their work was a continuation of both of their lines of research. Thus, Wannier had studied the theory of transition points under Fowler in Cambridge<sup>139</sup> and had attempted to apply the Bethe method to the melting process just before he began collaborating with Kramers in Utrecht in 1939.<sup>140</sup> Kramers, according to Dresden (1988), had published two earlier papers on ferromagnetism, but I will consider only the first of these two, which he published with G. Heller in 1934, in which they examined whether a classical system of spins can show spontaneous magnetization.<sup>141</sup> They focused on a particular model whose energy is a function of the spins and whose "classical" part treats the spin operator as a classical quantity.<sup>142</sup> They found that it displays a ferromagnetic transition for three-dimensional lattices (but not for lower-dimensional ones) and thus concluded that ferromagnetism can occur in a classical framework.<sup>143</sup>

<sup>136</sup> *Ibid.*, pp. 710–711.

<sup>137</sup> *Ibid.*, p. 711.

<sup>138</sup> Kramers and Wannier (1941a) and (1941b).

<sup>139</sup> Hoddeson, Schubert, Heims, and Baym (1992), p. 529.

<sup>140</sup> Wannier to Kramers, March 7, 1939, Archive for History of Quantum Physics, Niels Bohr Archive, Copenhagen, and other repositories.

<sup>141</sup> Heller and Kramers (1934); Dresden (1988), p. 29. The second paper was on series expansions of the free energy in the Heisenberg model; see Kramers (1936); ter Haar (1998), pp. 75–81.

<sup>142</sup> Thus, there is no conflict with the theorem of Bohr and van Leeuwen, which states that no magnetism can appear in classical systems.

<sup>143</sup> Dresden (1988), p. 29.

Kramers probably had given the Lenz-Ising model some thought well before Wannier started to work on it in 1939.<sup>144</sup> A footnote in their first paper<sup>145</sup> indicates that it was written by Wannier owing to wartime-communication difficulties while Kramers seems to have participated in the writing of the second one. Both dealt with transition points in and statistical theories of cooperative phenomena, specifically applying Boltzmann's formalism to them. They remarked that it "is generally believed" that transition points are a consequence of statistical theories, but this was "by no means immediately obvious,"<sup>146</sup> since they had been proven to exist only in condensing vapors. Their general aim thus "was to make statistical methods available for the treatment of cooperational phenomena,"<sup>147</sup> but they restricted their treatment to the special case of Curie points in ferromagnetism. Their purpose in treating ferromagnetism statistically was twofold:

The problem has a mechanical and a statistical aspect. On the mechanical side we wish to improve our understanding of the responsible coupling forces. On the statistical side we wish to derive with certainty the thermal properties from a reasonable accurate mechanical model.<sup>148</sup>

Kramers and Wannier acknowledged that quantum theory was able to explain "satisfactorily the origin and nature of the coupling forces"<sup>149</sup> and that some theories of ferromagnets can explain their thermal behavior in terms of them:

Not one, however, applies just straight statistics to the mechanical data. . . . Generally some simplifying assumption is introduced to facilitate the evaluation of the partition function. It follows that the results obtained are not necessarily a consequence of the mechanical model, but may well be due to the statistical approximation.<sup>150</sup>

Peierls had expressed a similar concern already in 1934:

Weiss's theory of ferromagnetism and analogous theories for other phenomena are approximately correct even in that domain [near the Curie point]; but in those cases the type of behaviour at the transition point is basically determined by the approximating assumptions which have to be made in order to simplify the theory. Such methods are therefore very useful for the description of systems whose qualitative behaviour at the transition is already known experimentally, but they are of no help in a theoretical investigation of the transition point itself.<sup>151</sup>

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<sup>144</sup> Wannier to Kramers, March 7, 1939, AHQP.

<sup>145</sup> Kramers and Wannier (1941a), p. 252.

<sup>146</sup> *Ibid.*

<sup>147</sup> *Ibid.*

<sup>148</sup> *Ibid.*

<sup>149</sup> *Ibid.*

<sup>150</sup> *Ibid.*

<sup>151</sup> Peierls (1934), p. 137.

Kramers and Wannier accepted that quantum theory is the fundamental theory of ferromagnetism, but their wish to treat ferromagnetism without any approximation prompted them to examine the Lenz-Ising model:

The present paper is an attempt to gain sound statistical information about some model of a ferromagnet. The Ising model has been chosen because its extreme simplicity makes it particularly suitable for such a purpose.<sup>152</sup>

Moreover, Peierls's rigorous proof that spontaneous magnetization can occur in the two-dimensional Lenz-Ising model made it reasonable to "suspect"<sup>153</sup> that a single transition point exists in it. They reasoned as follows. On the one hand, we know that at high temperatures thermal agitation destroys any ordering of the elementary magnets, so spontaneous magnetization vanishes completely in that temperature range. On the other hand, Peierls proved that spontaneous magnetization is nonzero at low temperatures. Nothing, however, is known about the behavior of spontaneous magnetization in the intermediate temperature range. Specifically, it was not known if the magnetization vanished completely at a definite intermediate temperature, "which is the standard idea associated with the Curie temperature,"<sup>154</sup> so Peierls's proof, while insufficient to rigorously infer the existence of a Curie point, makes it natural to suspect its existence: "It follows that the two-dimensional Ising model is a fair test case for the general statistical theory of ferromagnets."<sup>155</sup> Kramers and Wannier's approach,<sup>156</sup> in contrast to Peierls's proof, was much more mathematically involved and time-consuming: Wannier's letters to Kramers show that he worked on the problem for more than a year, at times very intensively.

At some point, Kramers and Wannier found it convenient to study the Lenz-Ising model in the absence of an external magnetic field. This strategy simplified the mathematics considerably, but it precluded the possibility of obtaining an expression for its magnetization. However, they took an important step (Wannier's letters to Kramers seems to indicate that this was Wannier's idea<sup>157</sup>), shifting from calculating its magnetization to calculating its energy and specific heat, which, since they "show singularities concurrently with the magnetization at the Curie point,"<sup>158</sup> a Curie point might appear in their temperature dependence even at zero magnetic field. An analysis of them thus would reveal the thermal behavior of the Lenz-Ising model, at least in principle.

Kramer and Wannier reformulated the problem of determining the partition function as one involving what later was called *transfer* matrices (which were independently

<sup>152</sup> Kramers and Wannier (1941a), p. 252.

<sup>153</sup> *Ibid.*, p. 256.

<sup>154</sup> *Ibid.*, p. 264.

<sup>155</sup> *Ibid.*, p. 256.

<sup>156</sup> ter Haar (1998), pp. 81–88, has an accessible description of the technicalities of their derivation.

<sup>157</sup> Wannier to Kramers, June 30, 1939, AHQP.

<sup>158</sup> Kramers and Wannier (1941a), p. 259.

employed by Montroll (1941) and Lassetre and Howe (1941)<sup>159</sup>). A transformation of the matrices showed that singularities in the temperature dependence appear in a high and a low temperature pair. There is one temperature,  $T_c$ , however, that did not pair with another temperature, which (in our notation) is given by

$$\sinh J/kT_c = 1. \quad (19)$$

Kramers and Wannier were not able to establish the existence of a Curie point, but they did establish that *if* one does exist, then it must be at the temperature  $T_c$  of Eq. (19), since it had to be a unique singularity, while all of the other singularities appeared in pairs. Their transformation method thus could not determine the nature of a possible singularity, that is, the behavior of the specific heat in the neighborhood of the Curie point, but it could be used to rule out some types of singularities. They proved by an exact derivation that if the energy is continuous at the transition point, then either the specific heat is also continuous at that point or it tends to infinity, and they used an argument based on numerics to show that it is in fact infinite at the Curie point. They compared none of their conclusions with experimental data on ferromagnets, but they criticized various approximations, including Kirkwood's, Bethe's, and a new one of their own. These fell into two classes. In the first, both the energy and the specific heat are found to be continuous functions of temperature, which presents a fundamental problem since the specific heat should be singular at the Curie point. In the second class, the energy is a continuous function of the temperature and the specific heat is discontinuous, but this behavior too is ruled out because the former contradicts the latter one. Thus, both classes of approximations are problematic.

Kramers and Wannier subscribed to the general view that the Lenz-Ising model was unrealistic,<sup>160</sup> but they opposed the general view that it was of no interest for the theory of ferromagnetism. They realized that it might provide insight into the theory of ferromagnetism and, more generally, into the nature of transition points: It could serve as a foundation for examining the validity of various uncontrolled approximations, and its exact solution might provide an example of a model that would yield a transition point. They thus evinced a balance between the realism and unrealism of the Lenz-Ising model, which was just what they required. They shared Francis Bitter's emphasis on exactness, but Bitter, unlike them, did not recognize this balance and did not focus on transition points.

Kramers and Wannier's mathematical methods played an important role in the subsequent development of the Lenz-Ising model, but I shall argue that their *attitude* towards it, as indicated above, was as significant to its future development. Their realization of its balance between realism and unrealism brought it "in from the cold," and to the attention

<sup>159</sup> Wannier (1945), pp. 50–51.

<sup>160</sup> They did not explicitly state how realistic a model of ferromagnetism they considered the Lenz-Ising model to be. Since their intention was to study "a reasonable accurate mechanical model" (p. 252), this statement must apply to the Lenz-Ising model. However, they acknowledged the existence of more correct theories of ferromagnetism, and four years later Wannier described the model as a "schematic representation" of ferromagnetism (and order-disorder phenomena in alloys for that matter); see Wannier (1945), p. 52.

of Lars Onsager. In this sense, Kramers and Wannier's work marks the beginning of the modern era of the study of the Lenz-Ising model, even though the excitement following Onsager's solution of the two-dimensional model in zero external field caused the number of publications on it to increase dramatically.

### *Onsager*

The Norwegian-born Lars Onsager (who became an American citizen in 1945) was a chemist with an unusual flair for mathematics and very broad interests in physics and chemistry. He had made valuable contributions to the theory of electrolytes and to the thermodynamics of irreversible processes (for which he received the Nobel Prize in Chemistry for 1968) and was trying to calculate the entropy of ice when Montroll informed him about his and Kramers and Wannier's results, which turned Onsager's attention to the Ising model.<sup>161</sup>

Onsager's pioneering contribution to the theory of phase transitions was his determination of the specific heat of the two-dimensional, zero-field Lenz-Ising model as a function of temperature in a closed form. He announced this result in the discussion following a paper that Wannier presented at a meeting of the New York Academy of Sciences in the spring 1942;<sup>162</sup> he published his derivation of it two years later (Onsager 1944). He followed up on this paper, which is notorious for its mathematical inaccessibility, by publishing a second one with Bruria Kaufman in 1947, which gives a simplified treatment of the mathematics (mainly due to Kaufman) but embodies the same physical content.

Onsager's realization of the mathematical intricacies of the description of transition points is evident in the very first sentence of his paper of 1944: "The statistical theory of phase changes in solids and liquids involves formidable mathematical problems."<sup>163</sup> Like Kramers and Wannier's, Onsager's focus was on transition points, but while Kramers and Wannier placed no further restrictions on their nature and almost exclusively discussed the Curie point, Onsager used Paul Ehrenfest's classification scheme to single out and concentrate on a general class of transitions. Its physical systems, which include the ferromagnetic transition, are characterized by no release of latent heat during the transition.

Onsager pointed out that this general class of transitions is comprised of several types of systems. For one type, the specific heat varies as  $(T_c - T)^{-1/2}$  and becomes infinite as the temperature  $T$  approaches the transition temperature  $T_c$ . This behavior is observed in the so-called  $\alpha$ - $\beta$  quartz transition in which quartz when heated changes quite rapidly from one solid form of quartz ( $\alpha$  quartz) to another form ( $\beta$  quartz). Onsager conjectured that this behavior "may be the rule for a great many structural transformations in

<sup>161</sup> Quoted in Hoddeson, Schubert, Heims, and Baym (1992), p. 531.

<sup>162</sup> Domb (1996), p. 130. Further information on how Onsager became interested in the problem and the origin of his mathematical ideas can be found in Domb's book, and in the various papers in Hemmer, Holden, and Kjelstrup Ratkje (1996) commenting on Onsager's work.

<sup>163</sup> Onsager (1944), p. 117.

crystals.”<sup>164</sup> For a second type, the specific heat at the transition temperature is finitely discontinuous, a feature exhibited experimentally by superconductors and theoretically by Bose-Einstein condensation. The Curie point of ferromagnetism and the transition of liquid helium to superfluid helium may be of the first type, because they both seem to be characterized by essential singularities, although it is not clear in both cases whether the singularities appear in the specific heat, as in the quartz transition, or in the first derivative of the specific heat with respect to temperature.

Owing to the very nature of such transitions, a crucial mathematical problem arises for systems characterized by an essential singularity: In computing the thermodynamic functions analytically by using a sequence of ever-better approximations, difficulties arise because the convergence of such a sequence is “notoriously slow”<sup>165</sup> when applied to a singularity and tends to become worse as it is approached. That suggested, Onsager wrote, that:

When the existing dearth of suitable mathematical methods is considered, it becomes a matter of interest to investigate models, however far removed from natural crystals, which yield to exact computation and exhibit transition points.<sup>166</sup>

That prompted Onsager to examine the Lenz-Ising model, because “[it] is known that this model should have a transition.”<sup>167</sup> Thus, like Kramers and Wannier, Onsager sacrificed the realism of the Lenz-Ising model for the sake of obtaining exact results.

Onsager, in contrast to Kramers and Wannier who maintained that the Lenz-Ising model represents a ferromagnetic crystal, was unconcerned about the specific system it represented, because his focus was on its ability to represent a particular kind of transition. He characterized it as follows:

The two-dimensional ‘Ising model,’ originally intended as a model of a ferromagnetic, [ref. to Ising (1925)] is known to be more properly representative of condensation phenomena in the two-dimensional systems formed by the adsorption of gases on the surfaces of crystals. [ref. to Peierls (1936a)].<sup>168</sup>

Whether Onsager saw it as a good representation of ferromagnetism in three dimensions is less clear, but three years later he and Kaufman returned to its physical representation as a ferromagnet, writing that, “The model may be called a crystalline ‘ferromagnetic’ with a scalar ‘spin’.”<sup>169</sup>

Setting aside Onsager’s exceedingly complicated mathematical methods in his 1944 paper,<sup>170</sup> he concentrated, as had Kramers and Wannier, on the specific heat of an “infinite [two-dimensional] crystal” lattice for the case of a vanishing field and found that

<sup>164</sup> *Ibid.*

<sup>165</sup> *Ibid.*, p. 118.

<sup>166</sup> *Ibid.*

<sup>167</sup> *Ibid.*

<sup>168</sup> *Ibid.*

<sup>169</sup> Onsager and Kaufman (1947), p. 139. Another two years later, Kaufman (1949) referred to the model as representing a binary alloy, the third of the three phenomena that Peierls had shown to be describable by equivalent models.

<sup>170</sup> Krieger (1996) gives an accessible outline of Onsager’s treatment.

the energy is continuous as a function of temperature but, further, that the specific heat goes to infinity as  $-\log |T - T_c|$  as  $T \rightarrow T_c$ , where  $T_c$  is given by Kramers and Wannier's equation (19). He showed that this result is at odds with the approximation used by Kramers and Wannier, which he considered to be the best one in the literature, by plotting the essential singularity of the exact result and showing its disagreement with the discontinuity they had found. This meant that all of the approximations used prior to 1944 were fundamentally incorrect.

Onsager did not confront his result with experimental data of any kind, which seems natural for problems such as ferromagnetism and alloys, since he solved the Lenz-Ising model only in two dimensions and that solution would likely differ in essential ways from that of three-dimensional problems. Wannier made this point in 1945 when he evaluated Onsager's result:

The detailed structure of our singularity. . . is not of . . . much significance. The logarithmic infinity of the specific heat, for instance, is probably due to the fact that the model is two-dimensional. It is not likely to show up in three-dimensional cases.<sup>171</sup>

That Onsager did not compare his result with experiments on the adsorption of gases on a solid surface, which is essentially a two-dimensional problem and one that he did consider the Lenz-Ising model to represent, does not seem to be as natural. This testifies to his focus on the mathematical intricacies of transition points rather than on the Lenz-Ising model as representing specific physical systems.

### *The role of mathematics*

The dramatic rise in the level of mathematics used in examining the Lenz-Ising model after Peierls's proof of 1936 warrants our attention. The application of the mathematical theory of matrices in the form of the transfer matrix played a crucial role not only in the work of Montroll, Kramers and Wannier, and Onsager, but also in that of Lassettre and Howe (1941). Kramers, according to his biographer, had used the idea that the partition function can be written as an eigenvalue of a matrix prior to Kramers and Wannier's papers,<sup>172</sup> but their papers contained "the first systematic and extensive application of matrix methods in statistical mechanics. . . ."<sup>173</sup> Prior to the advent of matrix mechanics in 1925, this highly efficient mathematical technique had not been part of most physicists' toolbox,<sup>174</sup> thinking that it belonged "exclusively to the realm of pure mathematics."<sup>175</sup> Thereafter, however, physicists became thoroughly acquainted with matrix methods and could apply their newly acquired mathematical skill to other areas in physics such as statistical mechanics, which was precisely what Kramers and others did. Kramers and Onsager, two of the protagonists in the development of the

<sup>171</sup> Wannier (1945), p. 58.

<sup>172</sup> ter Haar (1998), p. 6, quotes Uhlenbeck that Kramers "had found" the transfer matrix in 1937.

<sup>173</sup> Dresden (1988), p. 31.

<sup>174</sup> Jammer (1966), pp. 206–208.

<sup>175</sup> *Ibid.*, p. 207.



Lenz-Ising model between 1936 and 1944, probably learned the mathematical theory of matrices on their own since they received their formal education before the advent of matrix mechanics.<sup>176</sup> Wannier and Montroll, the other two main protagonists, who belonged to a later generation, probably did not since they received their mathematical training after matrices had become important in quantum theory.

These four scientists all shared a keen interest in mathematics and possessed extraordinary mathematical abilities,<sup>177</sup> but they seem to have differed in their attitudes towards mathematics. Onsager seems to have been the only one of the four who enjoyed abstract mathematics. Kramers, by contrast, “did not have much interest in the investigation of mathematical structures or in abstractions, generalizations, or axiomatizations,”<sup>178</sup> and although he had studied Hermann Weyl’s monograph, *Group Theory and Quantum Mechanics*, he deliberately avoided using group theory even in cases in which others found it natural to do so.<sup>179</sup> Onsager solved the Lenz-Ising model by using abstract mathematical methods involving quaternion algebras. Kramers’s hesitancy in using abstract mathematics might explain why he and Wannier were not able to solve the Lenz-Ising model, or why they were unable to achieve Onsager’s solution of 1944, but they may have been able to do something similar to what Bruria Kaufman did in 1947, namely, rewrite Onsager’s quaternion solution in terms of  $n$ -dimensional spinors. Wannier, in fact, had applied spinor algebra to the Klein-Nishina formula for Compton scattering already in 1935,<sup>180</sup> so he might in principle have been able to apply this mathematical theory to the Lenz-Ising model. Nevertheless, none of the other protagonists possessed Onsager’s extraordinary mathematical abilities and probably could not have solved the Lenz-Ising model. At the same time, the work of all four shows that statistical mechanics had become a mathematically demanding discipline by the 1940s.

### The post-Onsager era

The work of Kramers and Wannier and Onsager showed that the Lenz-Ising model was worthy of study as a model exhibiting transition points: Onsager and Kaufman noted

<sup>176</sup> Dresden is somewhat vague concerning the origin of Kramers’s knowledge about matrix theory, saying only that Kramers “either knew or rapidly mastered matrix techniques”; see Dresden (1987), p. 468. There is no account of the source of Onsager’s skills in matrix theory in the various biographical notes. However, it is likely that he acquired it on his own as he did other areas of mathematics, according to Longuet-Higgins and Fisher (1996), p. 10.

<sup>177</sup> Onsager received his Ph.D. degree in mathematics at Yale University; see Longuet and Fisher (1996), p. 19. For Kramers’s mathematical interests, consult Dresden (1987), pp. 466–470; Wannier’s is described in Anderson (1984), p. 101, and Hofstadter (1984), pp. 273, 275; information about Montroll is given in Shlesinger and Weiss (1985), p. 3.

<sup>178</sup> Dresden (1987), p. 467.

<sup>179</sup> *Ibid.*, pp. 468–469.

<sup>180</sup> Lacki, Ruegg, and Telegdi (1999), p. 478.

already in 1947 that by then this property had made it an object of intense study. Most of the papers dealing with it during the decade following Onsager's solution concerned five of its aspects:<sup>181</sup> (1) The application of Onsager's approach to other kinds of lattices;<sup>182</sup> (2) The determination of an expression for the spontaneous magnetization;<sup>183</sup> (3) The introduction of new methods that were mathematically equivalent to Onsager's, including simplifications of Onsager's approach;<sup>184</sup> (4) Attempts at generalization to the three-dimensional case; and (5) The introduction of new approximations.<sup>185</sup> Three new models also were introduced in the spirit of Kramers and Wannier and Onsager, that is, they were models with an emphasis on their mathematical amenability rather than on their physical realism.<sup>186</sup>

In all of these papers, the Lenz-Ising model was discussed almost exclusively for the purpose of obtaining a better understanding of transition points. In the 1940s and 1950s, however, divergent views arose as to what phenomena the model represents. Some, for instance, Domb (1949), Berlin and Kac (1952), Yang (1952), and Temperley (1956) maintained that it was a model of ferromagnetism, while others described it as representing binary alloys, and still others, such as Ashkin and Teller (1943) and Siegel (1951), did not attach it to any particular physical phenomenon but considered it to be a model of cooperative phenomena in general. Many of these people emphasized the importance of studying the model rigorously mathematically at the expense of its physical realism.

I will not discuss the reception and enormous influence of Onsager's solution on modern statistical physics,<sup>187</sup> but I will comment instead on how these new models illustrate how other physicists shared Kramers and Wannier's and Onsager's attitude towards models.

Julius Ashkin received his Ph.D. degree at Columbia University in 1943, a year before Onsager published his solution, and in a paper based on his thesis he and his supervisor Edward Teller proposed a generalization of the two-dimensional Lenz-Ising model. In the parlance of alloys, they defined it in terms of four different atoms instead of two as in the Lenz-Ising model, but they proceeded no further towards a concrete physical interpretation of it.<sup>188</sup> Their mathematical analysis mimicked Kramers and Wannier's, and for the case of attraction between similar atoms, they assumed the existence of a unique temperature singularity and were able to locate the critical point and determine

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<sup>181</sup> It is remarkable that several of the authors of papers on the Lenz-Ising model later became famous for their contributions to nuclear and elementary particle physics, areas quite different from the "crystal statistics" of the Lenz-Ising model. These include C.N. Yang, Y. Nambu, W. Lamb, and E. Teller.

<sup>182</sup> For instance, Newell (1950).

<sup>183</sup> Yang (1952).

<sup>184</sup> For instance, Nambu (1949).

<sup>185</sup> For instance, Kikuchi (1951).

<sup>186</sup> The models were described in Ashkin and Teller (1943) and Berlin and Kac (1952).

<sup>187</sup> For some aspects of this, see Brush (1983), pp. 244–246; Hoddeson, Schubert, Heims, and Baym (1992), pp. 528–533, 572–575, and Bhattacharjee and Khare (1995), pp. 816–821.

<sup>188</sup> This "neutrality" is reflected in the title of their paper: "Statistics of two-dimensional lattices with four components."

the behavior of the specific heat at that point. Like Kramers and Wannier and Onsager, they did not compare their model to any experimental results: Their focus was on its mathematical aspects rather than on its physical interpretation.

Theodore H. Berlin at Johns Hopkins University and Mark Kac at Cornell University together introduced two models in 1952, the Gaussian model and the spherical model,<sup>189</sup> both of which are continuum modifications of the Lenz-Ising model. They employed these models to investigate the nature of the ferromagnetic transition, which (as they noted in their introduction) presents great difficulties, as Onsager's solution shows. They endorsed Onsager's view of models:

We agree with Onsager that it is desirable to investigate models which yield to exact analysis and show transition phenomena. It is irrelevant that the models may be far removed from physical reality if they can illuminate some of the complexities of the transition phenomena.<sup>190</sup>

In 1964 Kac recalled how he and Berlin created their models. He had attempted to solve the Lenz-Ising problem in three dimensions but concluded that he could not do so, and "in the best mathematical tradition, not being able to solve the original problem, I looked around for a similar problem which I could solve."<sup>191</sup> That problem involved the determination of the partition function in the Gaussian model, so he designed this model to solve a mathematical problem, not to be physically realistic. Their spherical model was a continuation of this work, which they invented to remedy some of the mathematical shortcomings of the Gaussian model.

Berlin and Kac considered the spherical model to be the more realistic of the two, but they indicated their skepticism about its physical realism at the end of their paper:

The virtue of the spherical model of a ferromagnet is that its properties can be rather extensively discussed and that a three-dimensional lattice has ferromagnetic properties. It is of further interest that the model provides a classical mechanism for the Weiss phenomenological theory.

With respect to the physical ferromagnet, the model has nothing to say positively. We may briefly consider, however, the bearing of our results on the nature of the transition.<sup>192</sup>

Berlin and Kac thus continued the tradition of Kramers and Wannier and Onsager by focusing on the mathematical aspects of their models.

Ashkin and Teller were not so outspoken regarding the lack of physical realism of their model, but they detached their presentation of it from any physical phenomena it might represent, so they too seem to have followed in this same tradition. This illustrates the emergence of a new attitude among physicists towards models in statistical physics in which the exact mathematical solution of a new model was judged to be much more significant than its physical realism. That, of course, was not the *only* attitude physi-

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<sup>189</sup> Whereas Berlin was a physicist by training, Kac had a background in mathematics, an indication of the level of mathematical sophistication needed in the mathematical study of such models.

<sup>190</sup> Berlin and Kac (1952), p. 821.

<sup>191</sup> Kac (1964), p. 41.

<sup>192</sup> Berlin and Kac (1952), p. 827.

cists held after Onsager's solution, but it was one that was held by the highly influential physicists noted above.

In 1953 Newell and Montroll summarized the new attitude that physicists had adopted towards the Lenz-Ising model:

Actually the widespread interest in the model is primarily derived from the fact that it is one of the simplest examples of a system of interacting particles which still has some features of physical reality in it. The model forms an excellent test case for any new approximate method of investigating systems of interacting particles. If a proposed method cannot deal with the Ising model, it can hardly be expected to be powerful enough to give reliable results in more complicated cases.

Underlying the interest in this problem as a study of some physical model, there rests the more fundamental question. Does the formalism of statistical mechanics predict phase transitions and, if so, how? We can hardly give satisfactory answers to these questions without examples. Even an artificial example is better than none. So far only a few examples have been successfully studied. One of these is the famous Einstein-Bose gas condensation and another is Onsager's brilliant analysis of the two-dimensional Ising model. A third is the spherical model of cooperative phenomena. The model and not some mathematical approximation is in each case the sole cause of the phase transition represented mathematically by a singularity in some of the thermodynamic quantities.

Even though the Ising model is not considered to be a very realistic model of ferromagnetism, it is equivalent to a very good model of a binary alloy and an interesting model of a gas or liquid.<sup>193</sup>

### Discussion

Three questions deserve consideration. First, why did the Lenz-Ising model survive these tumultuous years between 1920 and 1950 despite the high odds that it simply would be forgotten? Second, is my claim correct that its development during this period was driven entirely by theoretical considerations and not by experimental results? Third, was the attitude of physicists towards the modelling process really as novel as I have claimed above?

Brush (1967) has suggested that the use of the Lenz-Ising model (or its mathematical equivalent) in the field of alloys may have saved it from oblivion. It was studied thoroughly in this field, as we have seen, and important results were obtained. However, if with Domb (1996) we accept the reasonable assumption that it owes its prominent place in modern physics to Onsager's solution because it displayed its potential in such an important area as critical phenomena, the picture becomes somewhat different, since that raises the question of Onsager's motivation. His solution was inspired by the mathematical results of Lassetre and Howe (1941) for alloys, and of Kramers and Wannier

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<sup>193</sup> Newell and Montroll (1953), pp. 353–354.

(1941a, 1941b) for ferromagnetism and transition points. Onsager (1971) commented on his inspiration in light of Kramers and Wannier's work:

He [Elliott Montroll] brought the news of this development on the Ising model, that Wannier had brought home from Holland after working with Kramers. Well, this intrigued me considerably; by that time the methods they had been using were a little more advanced than the ones I'd been playing with, which got very near to using a transfer matrix.<sup>194</sup>

Onsager thus was already trying to solve the Lenz-Ising model when he heard about Kramers and Wannier's work, which suggests that his work should not be seen as a direct continuation Kramers and Wannier's or Lassetre and Howe's. His reasons for studying the Lenz-Ising model may well have been different from those of his predecessors. I shall argue that since Onsager was mainly interested in describing transition points of continuous transitions, and was not concerned with alloys or ferromagnets, his focus on transition points was responsible for its survival. Onsager no doubt was aware of Peierls's proof that the Lenz-Ising model shows nonzero spontaneous magnetization at zero temperature in two dimensions. I therefore claim that it was rescued from oblivion because of Peierls's proof in combination with Onsager's (and secondarily of Kramers and Wannier's) interest in a mathematical description of transition points, and not, as Brush (1967) suggested, because of developments in the field of alloys.

Several other physicists shared Onsager's, Kramers's, and Wannier's interest in transition points beginning in the 1930s: Paul Ehrenfest published his famous classification of phase transitions in 1933, and Lev D. Landau published his famous theory of phase transformations in 1937 (although he announced it in 1936).<sup>195</sup> Why did they and other physicists become interested in transition points then? One explanation is that following the creation of quantum mechanics in the 1920s, physicists turned to other areas of research in the 1930s, one attractive area being the study of transition points since a large body of experimental results on diverse systems exhibiting transition points was being accumulated. Moreover, as exemplified by cooperative phenomena, physicists realized that these diverse systems shared certain characteristic features and could be classified accordingly. Thus, not only was there a host of experiments that required explanation, a new classification scheme had to be understood as well. Transition points also gave rise to significant theoretical concerns: Approximations had to be involved to treat the various models or theories, so were these approximations responsible for the existence of transition points or were they a consequence of the models or theories? And, was it possible for the Gibbs partition function to exhibit a discontinuous transition point?<sup>196</sup> These must have seemed to be fundamental questions at the time.

The physical interpretation of the Lenz-Ising model and the reasons for its study, as we have seen, changed considerably between the time that Lenz and Ising proposed it and when it was used in the context of cooperative phenomena. Comparisons to experimental results were almost absent during this period, except that in the context of ferromagnetism the model should show spontaneous magnetization or, in the theory of cooperative

<sup>194</sup> Onsager (1971), p. xxi.

<sup>195</sup> Hoddeson, Schubert, Heims, and Baym (1992), pp. 510–511, 522–523.

<sup>196</sup> Dresden (1988), p. 30.

phenomena, it should exhibit a transition point. But if its development was not a response to experimental results, what was the reason for it?

Even initially its development was not driven by discrepancies between the model and experiments. Lenz and Ising realized that Weiss's theory, which was based on the hypothesis of a molecular field, was able to explain a number of experimental results on paramagnetic and ferromagnetic materials; instead, they raised theoretical objections to Weiss's theory. Lenz criticized Weiss's assumption of free rotatability, arguing that it was not compatible with current theories of solids. They (and others) found the hypothesis of a molecular field formally acceptable, but not theoretically satisfactory owing to the absence of a physical explanation for it. To remedy this deficiency, they proposed a model based on what they considered to be more correct assumptions. Thus, Lenz gave a careful and complex argument for one of its basic assumptions that involved observations, the old quantum theory, and the theory of solids, while Ising did not give much of an argument for its other basic assumption but on the basis of both attempted to construct a simple model to explain ferromagnetism. Nonetheless, Ising himself admitted that it failed to display basic properties of ferromagnetism. His erroneous extension of his result to three dimensions seems to have been dismissed by some of his contemporaries, such as Pauli and Heisenberg.

After the creation of the new quantum theory in 1925, the elementary magnets in the Lenz-Ising model were reinterpreted as arising from the spin angular momentum of the electrons instead of their orbital angular momentum – a move that was possible because the model does not depend on the detailed properties of the elementary magnets. It then turned out that the model violated a fundamental principle of the new quantum theory, noncommutativity. Moreover, when it was compared to the more realistic Heisenberg model, it fell short and was rejected as a realistic model of ferromagnetism. Ising's conclusion that it was unable to explain ferromagnetism, however, seems not to have played an important role in its rejection; instead, its negative reception seems to have been shaped by its conflict with the new quantum theory and a desire to find a more realistic model.

The most striking change in the early fortunes of the Lenz-Ising model, however, probably was the increase in interest in it in the late 1930s and early 1940s concurrently with the decrease in interest in it as a model of ferromagnetism. I described the increasing interest in transition points in the 1930s and argued that the reason for the increasing interest in the Lenz-Ising model was physicists' realization that a more general theory of cooperative phenomena presented formidable mathematical difficulties. Because it was known to exhibit a transition point, which was the focus of interest in studying cooperative phenomena, its exact mathematical treatment became *en vogue* as a means of checking that its transition point arose from its intrinsic properties and not from the particular approximations employed in its analysis. This new motivation had significant implications. Even though physicists recognized that the Lenz-Ising model was, as Onsager wrote, "far removed" from real materials, and even though they acknowledged that it was less realistic than the Heisenberg model, they also realized that precisely because it struck a balance between realism and unrealism, it could be put to good use. Thus, whether or not the degree of its realism was deemed important depended upon the specific purpose physicists had for studying it. They did not consider it to be of much use in capturing the behavior of ferromagnetic materials, but

they regarded it of great interest for studying transition points and the mechanisms that generate them.

Is this attitude of physicists towards models really new? One could argue that Kramers and Wannier's and Onsager's attitude towards the Lenz-Ising model did not differ much from that adopted by nineteenth-century physicists toward models in kinetic theory.<sup>197</sup>

Stephen G. Brush has shown that in the nineteenth century physicists devoted much attention to the problem of computing observable properties of gases from their constituent molecules. Thus, James Clerk Maxwell (1831–1879), in his second kinetic theory of gases of 1866<sup>198</sup> (I will return to his first theory shortly), assumed that gas molecules are point-like and repel each other with an inverse-fifth power law of force, first, because all other force laws did not predict that the viscosity is proportional to the absolute temperature, which was thought to be the case experimentally, and second, because it greatly simplified the mathematical treatment. That was significant because, in modern parlance, it enabled him to calculate the desired transportation coefficients without having to know the velocity-distribution function explicitly.

It is not clear to me in reading Maxwell's paper which of these two reasons was the more important to him,<sup>199</sup> but if we assume for the sake of argument that he chose the inverse-fifth power law because it simplified the mathematical treatment, then we might ask: How did Maxwell's approach in his kinetic theory differ from that of Kramers and Wannier and Onsager in analyzing the Lenz-Ising model? Was not an ideal system chosen in both cases for the same reason? I suggest that the fundamental difference was that Maxwell's idealization did not violate a more fundamental molecular theory at that time, while Kramers and Wannier and Onsager knew that the Lenz-Ising model was in conflict with Heisenberg's fundamental theory of ferromagnetism.

Maxwell presented his first kinetic theory at a Meeting of the British Association in 1859 (it was published in the *Philosophical Magazine* in 1860), in which he assumed, as others had before him, that gas molecules behave like billiard balls and undergo elastic collisions.<sup>200</sup> He broke with this assumption in his second theory of 1866, but he continued to use his first theory (at least once, in 1873). Moreover, his contemporary Oscar E. Meyer accepted and stuck to the billiard-ball model even after Maxwell's second theory appeared, and when a discrepancy arose between it and experiment, he suggested that the internal structure of the gas molecules should be taken into account.<sup>201</sup> In sum, Maxwell could not violate a fundamental theory because there was none at the time to violate, whereas Kramers and Wannier and Onsager deliberately violated a fundamental physical theory.

The study of the Lenz-Ising model was not the only cause for the increasing focus on mathematical models in statistical physics. Developments in the theory of gas con-

<sup>197</sup> I am grateful to an anonymous reader for posing this question on the difference between these attitudes.

<sup>198</sup> Published as Maxwell (1867).

<sup>199</sup> In his writings, Brush seems to weigh the reason of the mathematical simplicity higher than the reason concerning the compatibility with experiments; see, for instance, Brush (1966), p. 5; and Brush (1983), pp. 206–207.

<sup>200</sup> See, for instance, Brush (1983).

<sup>201</sup> Brush (1976).

densation, initiated by Joseph E. Mayer and pursued by George Uhlenbeck, Boris Kahn, and others,<sup>202</sup> may have been equally or even more important in this trend. Kramers and Wannier mentioned that the theory of gas condensation was the only theory in which physicists had attempted to prove that the existence of a transition point follows from a statistical treatment. Nevertheless, Onsager’s proof that the Lenz-Ising model offered the possibility of a mathematical treatment of ferromagnetism surely reinforced this trend. At the very least, the development of the Lenz-Ising model played a significant role in the emergence of mathematical models in statistical mechanics.

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<sup>202</sup> Brush (1983).



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# 5

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## Summary of Part I

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This part of the dissertation has dealt with the roots and early development of the Lenz-Ising model in terms of three phases: first, its proposal in the 1920s; second, the replacement of foundational theory (from the old quantum theory to the new quantum mechanics) and the subsequent change in perception of the model; third, the growing interest in the model in the late 1930s to the 1940s, but now as a model of transition points in general rather than of ferromagnetism only.

In addition to introducing the Lenz-Ising model, describing its historical roots, recounting how mathematically equivalent models appeared within cooperative phenomena, and charting the technical development which led from Peierls's proof that the model exhibits a non-zero spontaneous magnetisation to Onsager's solution, this part contributes to the overall conceptual scheme of the dissertation. More precisely, it shows that both the perception of the Lenz-Ising model and the role the model can play changed in the epoch from 1920 to 1950. Moreover, it reveals some of the driving forces behind these changes. These points will briefly be touched upon in the following.

The change in the perception of the model as a representation of ferromagnetism from Lenz and Ising to Heisenberg, Pauli and others, can be ascribed to the change in the foundational theory which was caused by the replacement of the old quantum theory with the new quantum mechanics. All of a sudden Lenz's assumption was invalid because spins are not restricted to behave the way he had assumed. In an environment mainly interested in models that are well-founded in terms of the new quantum mechanics, the Lenz-Ising model was considered to be of mere mathematical interest because of its distorted representation of the spins. So, the change in the perception of the Lenz-Ising model due to the change in the views on its realism altered the role that the model was able to play – it was no longer perceived as relevant for the modelling of ferromagnets.

The growth in the interest in the model in the late 1930s-early 1940s was a combination of the realisation that the mathematical problems involved in the handling of cooperative systems are large, with a wish to show that the formalism of statistical mechanics is capable of accommodating a phase transition. In this situation *any* model which could be treated mathematically and which was likely to exhibit phase transitions, was found to be interesting. So, the change in the interest in the model was not due to a shift in the perception of the model's ability to represent physical phenomena – everybody agreed that it was unrealistic – but to the emergence of a new view on the *role* of the model.

In other words, the answer to the first issue of section 1.1 is that the replacement of the foundational theory did indeed change the perception of the Lenz-Ising model. Moreover, the model was not considered to be of much worth for a discussion of ferromagnetism. It required a change in the role of the model to generate a renewed interest in it.



## **Part II**

# **From Irrelevant to Prominent Model: 1950–1970**





# 6

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## Introduction to Part II

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By the end of the 1960s the Lenz-Ising model in its various guises had become one of the most important models for understanding so-called critical phenomena. In this decade, the term critical phenomena emerged as an umbrella term for the transition points of a range of physically disparate phenomena. The transition points of ferromagnetism, antiferromagnetism,<sup>1</sup> binary alloys, and the critical point of gas condensation, were of particular importance – I shall denote them the core areas of critical phenomena.

In the 1950s it was not at all in the cards that the Lenz-Ising model should be the predominant model of critical phenomena, and most physicists perceived the model as physically irrelevant: it could be used to show that statistical mechanics allows for phase transitions, but the model was judged incapable of giving insight into real physical systems. However, by the end of the 1960s, the model had acquired a position as a prominent model of critical phenomena. What had happened? Why had the Lenz-Ising model changed status? I shall answer these questions by first providing answers to two other questions. First, why did the model become physically relevant?

Around the time of Onsager's solution in 1944, the Lenz-Ising model was mainly used as a proof by example that the formalism of statistical mechanics is able to exhibit a phase transition. Immediately after the advent of Onsager's solution, the model also played a part as a test of approximative methods interesting for more physically relevant models. These methods were applied to the two-dimensional Lenz-Ising model and were confronted with Onsager's solution for this model. However, the model was perceived to be too far removed from real systems to be able to say anything about their behaviour. In short, the Lenz-Ising model was a toy model in the sense of section 2.3.1.

The first question can then be reformulated as follows: why was it realized that the Lenz-Ising was able to provide insight into real systems? Perhaps expectedly, the answer to this question is that it was realized that the model is in surprising agreement with certain experimental results. However, since it did disagree with some other important experimental results, most notably in the area of ferromagnetism, the picture is somewhat blurred and confusing and there still seems to be some explaining to be done.

When it is established why the model was found to be able to represent real systems, my second question is why the model acquired the prominent position it did and to what extent it toppled other models in the area of critical phenomena. In the 1950s, the most prominent models for three of the four core areas of critical phenomena were not the Lenz-Ising model. In the area of liquid-gas by far the most important model was the so-called Mayer model, while the (generalised) Heisenberg model was perceived to be the best model of ferromagnetism and antiferromagnetism. In the 1960s, the Mayer model was toppled by the Lenz-Ising model, while it had roughly the same status as the Heisenberg

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<sup>1</sup>Antiferromagnetism is perhaps a little unfamiliar to the reader. While the spins of a *ferromagnet* tend to align in parallel below the Curie point, for an antiferromagnet they prefer an arrangement where neighbouring spins are antiparallel below the transition point, which here is called the Néel point.

model in the 1950s. Why did most physicists use the Lenz-Ising model in the 1960s rather than those two models of the 1950s? This is the question of the Chapter 9.

The question of Chapters 10 and 11 is how the Lenz-Ising model was more precisely used to get insight into critical phenomena. In fact, I shall show that the approach to modelling which grew out of the use of the Lenz-Ising model in the 1960s represents a radically different approach to the modelling process than did the previous ones which had their hey days in the 1950s. This is the topic of Chapter 12, which deals with what I have called modelling approaches.

## 6.1 Cooperative Phenomena and Critical Phenomena

In order to appreciate the history of the Lenz-Ising model, it is necessary to place it within some other developments. As described in the previous part of this dissertation, the model was mainly used as a prototype of *cooperative phenomena* in the 1930s and 1940s. These phenomena can only be described properly by taking the cooperation between their constitutive units into account. The types of phenomena subsumed under this umbrella are very varied and include various phase transitions etc. The few physicists interested in the model in the 1950s, perceived it, as we shall see, as a model of cooperative phenomena. In the 1960s, the model was seen mainly as a model of critical phenomena (see Chapter 2 for a description of some of these phenomena), a subclass of cooperative phenomena. This behaviour was typically described in terms of critical point exponents, which were of central importance to the theory. Mathematically speaking, if a function behaves as  $x^b$  for  $x \rightarrow 0^+$ , which we shall write as

$$f(x) \sim x^b \text{ for } x \rightarrow 0^+, \quad (6.1)$$

the exponent  $b$  is given by

$$b = \lim_{x \rightarrow 0^+} \frac{\ln f(x)}{\ln x}. \quad (6.2)$$

Such exponents are a convenient way of describing the singularities of the system, but they contain considerably less information than the complete form of the function. This means that correction terms are needed in order to get the entire behaviour. Several types are compatible with equations 6.1 and 6.2, for instance the following ugly expression:<sup>2</sup>

$$f(x) = A |\ln |\ln x||^\mu x^b (1 + a(\ln x)^{-\nu} + \dots). \quad (6.3)$$

Here I shall briefly touch upon three aspects of cooperative phenomena and critical phenomena which were important prior to the epoch under study and played significant roles in this epoch.<sup>3</sup>

*Mean-field theories*<sup>4</sup> were and are an important tool for the examination of models. In a mean-field description one replaces the direct interaction between the individual constituents by a uniform, average field – the mean-field – which is the same for all constituents. For instance, for a magnetic model, the pairwise interaction between spins is replaced by a field taken to be proportional to the total magnetisation of the model. The

<sup>2</sup>I got this nice example from Fisher (1967), p. 623.

<sup>3</sup>A comprehensive account can be found in Hoddeson, Shubert, Heims and Baym (1992), pp. 518-533, pp. 572-584.

<sup>4</sup>For a description of mean-field theories, see Binney et al. (1992), pp. 158-177.

total field experienced by every spin is the sum of the mean-field and the external field. This is the Weiss theory of a ferromagnet. Other typical examples of mean-field theories are the van der Waals theory of gases<sup>5</sup> and the Bragg-Williams theory of an alloy. Rather than a ‘real’ theory, a mean-field theory is a technique for dealing approximately with models. Instead of treating the interactions between the constituents of the model correctly, these interactions are approximated by a mean-field. One can, for instance, talk about the mean-field theory of the Lenz-Ising model.

The three mean-field theories just described – Weiss, van der Waals, and Bragg-Williams – apply to different phenomena, but they give values of exponents which are identical for analogous properties of the three systems. Moreover they are *independent* of dimension. The most important results are:<sup>6</sup>

- The specific heat makes a *finite jump* at the critical point.
- The coexistence curve of the van der Waals gas is parabolic, i.e., the difference between the volume of the gas  $V_g$  and that of the liquid  $V_l$  is given by

$$V_g - V_l = A(T_c - T)^{\frac{1}{2}}, \quad (T \rightarrow T_c^-). \quad (6.4)$$

Here  $T$  is the temperature,  $T_c$  is the critical temperature and  $A$  is constant. For a Weiss ferromagnet, the magnetisation is a parabolic function of the temperature.

- The compressibility of the van der Waals gas

$$\kappa_T = -\frac{B^\pm}{|T - T_c|}, \quad (T \rightarrow T_c^\pm), \quad (6.5)$$

where  $B^+$  and  $B^-$  are constants for the regions above and below the critical temperature, respectively. The susceptibility  $\chi$  of the Weiss ferromagnet behaves in a similar manner.

From the modern point of view, the problem with mean-field theories is that they neglect fluctuations. Since fluctuations are important at the critical point, this is a serious objection. This was not recognised at first, but when the results of a mean field theory treatment of the two dimensional Lenz-Ising model were compared with Onsager’s solution, the former were found to be qualitatively wrong.

Two other developments need to be mentioned. Mainly for terminological reasons a classification by Paul Ehrenfest in 1933 is relevant for the following discussion. In 1933, he proposed a taxonomy of general types of phase transitions according to their thermodynamic behaviour: A phase transition is of the  $n$ th order if the  $n$ th derivative of the free energy with respect to any of its arguments is continuous at the phase transition. The Ehrenfest classification was inspired by the 1932 discovery of a jump discontinuity in the specific heat of liquid helium at the lambda transition where liquid helium undergoes a transition from a normal fluid to a superfluid. However, even after it was realised in the 1950s that liquid helium actually exhibits a divergence in the specific heat at the lambda transition, Ehrenfest’s classification prevailed. It was not unusual in the epoch under study to talk about first and second order transitions; critical phenomena were thought to be of second order. With the realisation that generally thermodynamic quantities actually

<sup>5</sup>In the standard derivation by Ornstein, rather than in van der Waals’s own. See Domb (1996), p. 47.

<sup>6</sup>See Uhlenbeck (1966).

diverge as the critical point is approached, it became common to classify phase transitions as either first order or continuous.<sup>7</sup>

The other development is a theory by Lev Landau of 1937 on the thermodynamics of phase transitions.<sup>8</sup> The aspect of this theory of relevance here is the fundamental assumption that the thermodynamical free energy of a system can be Taylor-expanded in a suitable variable at the critical point. Theories based on this assumption are sometimes called *phenomenological theories*. This assumption, which looks innocent, does in fact lead to the same predictions as in the mean-field theories. The fact that the mean-field theories and the phenomenological theories lead to the same critical behaviour is the basis for subsuming these two apparently different approaches under the heading ‘classical theories.’<sup>9</sup> Here ‘classical’ is used as meaning ‘conventional’ rather than non-quantum mechanical. As we shall see, the examination of the validity of such classical theories became a major research issue in the treatments of critical phenomena in the 1960s.

### 6.1.1 The Heisenberg Model

For future reference, it is worthwhile to discuss the Heisenberg model briefly. In the quantum mechanical Heisenberg model, the quantum mechanical exchange forces can be represented by the following term in the Hamiltonian:

$$J\mathbf{s}_i \cdot \mathbf{s}_j = J(s_{xi}s_{xj} + s_{yi}s_{yj} + s_{zi}s_{zj}). \quad (6.6)$$

Here,  $s_{xi}$ ,  $s_{yi}$ , and  $s_{zi}$  are non-commuting operators which represent the components of spin  $i$  (and similarly for spin  $j$ ). The spin of magnitude  $s$  can take on  $2s + 1$  orientations. Because of the non-commutative property of the spin operators the quantum mechanical Heisenberg model is difficult to handle. In order to circumvent this difficulty, the model is simplified by replacing the term above with

$$J\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j. \quad (6.7)$$

Here,  $\boldsymbol{\sigma}_i$  and  $\boldsymbol{\sigma}_j$  are unit vectors allowed to assume all orientations in three-dimensional space. This model can be considered, properly normalised, to be the  $s \rightarrow \infty$  limit of the quantum mechanical Heisenberg model where the spins are allowed a continuum of orientations.<sup>10</sup> This model is called the *classical* Heisenberg model. It was studied by Heller and Kramers in 1934 in the low-temperature domain.<sup>11</sup>

In 1930, Felix Bloch discovered an interesting phenomenon in the Heisenberg model: spin waves.<sup>12</sup> At absolute zero, the spins of the model will all be aligned in parallel. However, at non-zero temperatures, each spin can deviate slightly from the ordered state of

<sup>7</sup>See Jaeger (1998) for a historical account of this classification.

<sup>8</sup>Nielsen and Timmermann (2002).

<sup>9</sup>See, e.g., Fisher (1965).

<sup>10</sup>Stanley (1971) wrote in 1971:

[...] it is only within recent years that it has been realized that the classical model is an extremely realistic approximation to the quantum-mechanical case for temperatures near  $T_c$  [...]. It is now believed that critical point indices are either independent of spin quantum number  $S$  or they depend on  $S$  so weakly that to an extremely good approximation the spin dependence may be neglected. Hence, although the classical Heisenberg model is an unrealistic approximation to the quantum-mechanical case in the low-temperature domain, it is extremely realistic in the neighbourhood of  $T_c$  as regards critical indices. (Stanley; 1971, p. 112)

<sup>11</sup>Heller and Kramers (1934).

<sup>12</sup>Hoddeson, Baym and Eckert (1992).

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total alignment. In a concerted effort of a large number of spins all these small deviations will add up and form a wave-like pattern, a spin wave. Since the formation of a spin wave requires small deviations of the spin, it will not occur in the Lenz-Ising model – this model is too crude. However, for Heisenberg model such spin waves are important, because in some situations they can destroy the occurrence of ferromagnetism in the model and their theoretical investigation have subsequently played an important role within the area of magnetism.



# 7

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## The Attitudes Towards the Lenz-Ising Model in the 1950s

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In the first part of the dissertation, I have shown that in the second half of the 1940s and the early 1950s, the Lenz-Ising model was not considered to be a good representative of ferromagnets due to its lack of realism. The model was examined mathematically, but with the purpose of enabling an investigation of the approximation methods applied to other models.

In this chapter I shall examine the attitudes towards the model in the 1950s. The findings of this examination are mainly to be used in the following chapters to discuss the change in the perception of the Lenz-Ising model within the field of critical phenomena. Therefore I shall examine somewhat slavishly the perception of the model in the four core areas of what was to be known as ‘critical phenomena’ in the 1960s. My main point will be that the model was, by and large, dismissed as a representation of ferromagnetism, antiferromagnetism and gas condensation (in terms of the so-called lattice gas model; see section 7.1.2). On the other hand, the model was used to represent the order-disorder transition in alloys; in fact it was the preferred model within this area, the last of the core areas. The mathematical investigations of the model continued throughout the 1950s, but I shall argue that this does not undermine the point just made.

One group, Cyril Domb’s at King’s College, London, seems to have held a different view on the model than did the rest of the physics community.<sup>1</sup> This group actually put a lot of efforts into examining the Lenz-Ising model in the 1950s, mainly as a model of ferromagnetism and antiferromagnetism. This makes it worthwhile to examine the reasons of Domb and co-workers for applying such strenuous efforts to this model in order to contrast it with the dismissive attitude of others at same time.

### 7.1 The Status of the Model in the 1950s

From recollections by several of the protagonists, it is clear that the Lenz-Ising model was perceived unfavourably as a model of physical phenomena in the 1950s. Cyril Domb has recalled about his time at the Clarendon Laboratory at Oxford in 1949–1952: “Elliott Montroll came to visit me at Oxford, he being one of the few people in the world interested in the Ising model at that time.”<sup>2</sup> In an interview conducted by S. S. Schweber in 2002, Domb elaborated: “The Ising model was not very popular at the time [i.e. the 1950s]: It was the Heisenberg model that was considered interesting. The Onsager solution was

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<sup>1</sup>Some Japanese physicists treated the model in the 1950s as a model of condensation, but since they do not seem to have received much interest from others, they will not be taken into account.

<sup>2</sup>Domb (1990), p. 15.



thought to be a mathematical curiosity. The order-disorder model was considered ‘real’.”<sup>3</sup>

The Chinese-American physicist Chen Ning Yang – who determined the magnetisation of the two-dimensional model in 1952<sup>4</sup> – has in several places recalled that the Lenz-Ising model was perceived as physically irrelevant. In his most sharp formulation, in 1995, he put it this way:

Young physicists today may find it surprising, even unbelievable, that in the 1950’s the Ising model and similar problems were not deemed important by most physicists. They were considered arcane exercises, narrowly interesting, mathematically seducing, but of little real consequence. There was the phrase [ref. to Pais (1958)], for example, of ‘contracting the Ising disease.’ In a recent article by Dyson in my *Festschrift* [...] he recalled how, in 1952, when he read my article about the magnetization of the Ising model, he was impressed by the beautiful complexity of the calculation and the beautiful simplicity of the result, but felt I was wasting my time. (Yang; 1995, p. 3)

Yang has also stated that some physicists thought it was only “a kind of interesting mathematical game, not to be taken seriously.”<sup>5</sup> In the reference by Abraham Pais cited by Yang, Pais wrote: “In 1952 Yang contracted the celebrated Ising disease, but unlike many of his fellow patients he pulled through by being able to compute the spontaneous magnetisation of the two-dimensional lattice [...]”<sup>6</sup> In the paper by Freeman Dyson referred to by Yang, Dyson wrote about the paper where Yang calculated the spontaneous magnetisation of the two dimensional Lenz-Ising model:

The result amazed us because of its beautiful simplicity; Frank’s [Frank is Yang’s nickname] calculation amazed us because of its beautiful complexity. The calculation was a virtuoso exercise in the theory of Jacobian elliptic functions. The result was a simple algebraic expression from which all traces of elliptic functions had disappeared. After working through this astonishing display of mathematical fireworks, I expressed some disappointment that Frank had chosen such an unimportant problem on which to lavish his skill. I remarked, with the arrogance of youth, that if Frank could ever do a beautiful job like this on a problem of major importance, then he would really amount to something as a scientist.<sup>7</sup> (Dyson; 1995, p. 131)

In the quotations by Yang, he referred to the opinion of others, but did he himself share their views at the time? He might have had a different opinion (after all, as noted above, he provided a result in 1952 on the two dimensional model, second only to Onsager’s in importance and of equal mathematical complexity). He is not clear on the issue of physical relevance, but he does not write that he disagreed in the 1950s with the prevalent statements about the irrelevance of the model, so it seems likely that he did share this view.

It is natural to ascribe the physicists’ dismissal of the Lenz-Ising model in the 1950s as due to their view that the model lacks realism. In the following, I shall document that in the core areas of critical phenomena, the model was indeed perceived as unrealistic, except for the case of alloys.

<sup>3</sup>Available at <http://hrst.mit.edu/hrs/renormalization/Domb/index.htm>

<sup>4</sup>Lars Onsager also accomplished this, but only published the formula, not the proof.

<sup>5</sup>Yang (1983), p. 13. He gave a similar assessment in Yang (1972), p. 3.

<sup>6</sup>Pais (1958), p. 299.

<sup>7</sup>For the sake of completeness it should be mentioned that Dyson continued with the statement that Yang’s work on non-Abelian gauge theory two years later revealed that Yang was a real scientist.

### 7.1.1 Attitudes within the Core Areas

In the field of ferromagnetism and antiferromagnetism, the *Heisenberg* model held a prominent position in the 1950s. One of the leading authorities on magnetism, John van Vleck wrote about the general state of the theory of ferromagnetism:

In contradistinction to superconductivity, the mechanism responsible for ferromagnetism is at present fairly well understood in broad outline. It is generally agreed that the exchange forces between electrons provide the coupling between the elementary magnets which is a prerequisite to ferromagnetism and which is so well represented empirically by the Weiss molecular field. (van Vleck; 1953, p. 220)

Van Vleck mentioned four models and the Lenz-Ising model was *not* one of them. The simple Heisenberg model ascribes one spin per atom:

I think it can be regarded as agreed that the simple Heisenberg theory is too crude, since the experimental values of the saturation magnetization show clearly that there is not an integral number of spins per atom. (van Vleck; 1953, p. 221)

Instead he preferred what he called the generalized Heisenberg model. This model allows a non-integral number of spins per atom by considering excited states of atoms in the crystal lattice.<sup>8</sup> So, van Vleck ranked the models representing ferromagnetism. In this ranking the (simple) Heisenberg model was once removed from the more realistic generalised Heisenberg model, which was not even a faithful representation of ferromagnetism. The Lenz-Ising model was even more removed from this model and it most unlikely that van Vleck would not subscribe to his statement of 1945 where he wrote that results for the Lenz-Ising model “should not be identified too closely with the actual magnetic behavior of the material simply because of the inadequacy and arbitrariness of the model.”<sup>9</sup>

Other physicists of the epoch shared this view of the Lenz-Ising model of ferromagnetism. Domb and Sykes (1957a) wrote: “[...] the Ising interaction can only be regarded as a valid approximation for substances exhibiting strong magnetic anisotropy [...]”<sup>10</sup> Dyson, in addition to his disinterest in Yang’s work on the Lenz-Ising model, considered the Heisenberg model to be more realistic than the Lenz-Ising model: “we may justifiably claim that our model [the Heisenberg model] has considerably greater similarity than the Ising model has to a real ferromagnet.”<sup>11</sup>

There is one area of magnetism where the Lenz-Ising model was perceived as a realistic model, namely that of extremely anisotropic materials. The availability of pure rare earth elements in the early 1950s “stimulated the study of new magnetic materials”<sup>12</sup> and in the late 1950s materials were discovered with special properties such that they meet

<sup>8</sup>Van Vleck gave this model the following assessment:

In summary, it may be said that the results of the present paper are discouraging, as the essence of what we have said is that the truth is somewhere between the collective electron model (b) and the generalized Heisenberg model (c), probably closer to (c) than (b). (van Vleck; 1953, p. 227)

<sup>9</sup>van Vleck (1945), p. 34.

<sup>10</sup>Domb and Sykes (1957a), p. 216.

<sup>11</sup>Dyson (1956), p. 1218.

<sup>12</sup>Wolf (2000).

the theoretical conditions for being ‘Ising-like.’ The most important of these conditions is that they should be anisotropic in such a way as to make them well represented by the anisotropic interaction of the Lenz-Ising model.<sup>13</sup> The first rare earth compound to be identified as ‘Ising-like’ was dysprosium ethyl sulphate.<sup>14</sup> This connection between the model and compound was established by Cooke et al. (1959), who argued for a “unusually strong coupling between the ions arising from magnetic dipole-dipole interaction”<sup>15</sup> and that the effect of other interactions is small. This means that at extremely low temperatures ( $\sim 0.1^\circ\text{K}$ ) the material “should closely resemble those of a classical Ising model with known, dipolar forces between the ions.”<sup>16</sup> However, even though other Ising-like materials were found, the most common ferromagnets did not meet the requirements for being of this type.

### 7.1.2 The Lattice Gas Model

In 1952 Tsung-Dao Lee and Yang introduced the word ‘lattice gas’ for a well-known model of a gas on a lattice. In this model each site of the lattice can be either vacant or occupied by one gas atom (multiple occupancy is not allowed).<sup>17</sup> Lee and Yang showed that this model is mathematically equivalent to the Lenz-Ising model of spins, meaning that there is an exact mapping of the partition function of one model into the other.<sup>18</sup> By associating energies to nearest neighbours – a pair of nearest neighbour atoms has negative energy, and both a pair of vacant sites and a pair of an atom and a vacant site have zero energy – the model mimics the attraction between atoms in for instance a monatomic gas (for a more mathematical statement of this model, see Appendix B). Lee and Yang were not the first to consider lattice theories of gases<sup>19</sup> nor to notice the correspondence between the two models,<sup>20</sup> but since they gave a systematic account and derived some new results, their paper is usually considered to be the origin of the lattice gas model.<sup>21</sup>

In the area of gas condensation, the lattice gas model held a position similar to its mathematical equivalent in the field of magnetism. For condensation the preferred model was a model by Joseph E. Mayer (see Chapter 9) and by and large the lattice gas model was not discussed as a realistic representation of gases. In his influential monograph of 1956 on phase transitions, H. N. V. Temperley (1956) included a chapter on evaporation and liquefaction where he referred to possible liquid models. His exclusion of the lattice gas model in this context exemplifies the general lack of interest in this model as a model of condensation.<sup>22</sup> The lattice gas model was not compared with experiments in the 1950s,

<sup>13</sup>See Wolf (2000) for a further discussion.

<sup>14</sup>Wolf (2000).

<sup>15</sup>Cooke et al. (1959), p. 246.

<sup>16</sup>Cooke et al. (1959), p. 246.

<sup>17</sup>Lee and Yang (1952).

<sup>18</sup>I shall not go into the details of how this is shown, as the proof can be found in many textbooks on statistical mechanics, e.g. Goldenfeld (1992), pp. 74-79.

<sup>19</sup>Henry Eyring applied such theories to the liquid state in the years 1936 to 1941. See Rowlinson and Curtiss (1951).

<sup>20</sup>In a letter to George E. Uhlenbeck, Joseph E. Mayer wrote on September 26, 1941: “I think there is a formal analogy between the condensation theory and the Kramers-Wannier treatment of the order-disorder phenomenon [that is the Lenz-Ising model]. Montroll seems to think so, but I believe the connection is fairly far-fetched.” MSS 47, Box 14, Folder 4, in Mandeville Collection, UC San Diego. See Brush (1967), p. 890, for some of the published work prior to Lee and Yang’s paper.

<sup>21</sup>Brush (1967).

<sup>22</sup>Another example is a recollection by Domb:

probably because there were exact results only for the two-dimensional variant (the series expansions, which were successfully applied to the magnetic Lenz-Ising model, were for some reason not applied to the lattice gas model).

### 7.1.3 Alloys

In the field of alloys, the Lenz-Ising model was in fact preferred to others. Even though some of the assumptions of the model were considered to be crude, the model had a reputation of being quite realistic here. Therefore, it is interesting to look more closely at the model within this area.

In his description of models, including the Lenz-Ising model, for the order-disorder phenomenon, Edward W. Elcock (1956) wrote that all existing treatments fulfil two fundamental assumptions. The first is that it is possible to divide the Hamiltonian into three terms: i) a term  $H_1$  representing a crystal of structure-less particles; ii) a term  $H_i$  which is a function of variables specifying the internal structure of the actual ions in the crystal; and iii) the term  $H_e$  which is a function of variables specifying the rest of the electrons moving in the potential of the ions. The term  $H_1$  can be subdivided into a kinetic and a potential part. The potential part is the sum of the energies for ions in their state of equilibrium  $c$ , denoted  $V(c)$ , and the potential energy arising from the displacement of ions from their equilibrium position. Elcock's next assumption is that it is only  $H_i$  and  $V(c)$  which depends on the configuration, so the energy of the other terms are constant for all configurations.

He wrote about the theoretical basis of these assumptions:

In actual fact, neither of the assumptions we have made can be rigorously true: there will in general be interactions between the various components (ions, electrons) of the crystal which make it impossible to specify rigorously the state of any one component without reference to the states of the other components; further – and of interest later – the normal modes of vibration and the electronic states of the crystal, given by  $H_1$  and  $H_e$ , will certainly depend in some way on the configuration of the crystal. In this kind of treatment we are considering here, however, it is assumed that neglect of such (possibly secondary) effects will not substantially affect the predictions of the treatment, which it is hoped will lead to results sufficiently in agreement with experiments to deepen our understanding of the phenomenon under investigation. It is also hoped that a careful examination of the differences between the predictions of the treatment and the results of experiment may indicate the importance of the approximations that have been made, and may suggest ways in which they can be improved. These expectations are, as will be seen later, in the main justified. (Elcock; 1956, p. 81-82)

After these assumptions about *all* the models, he continued with yet another assumption:

[ . . . ] it will be assumed that the configuration energy may be written as a sum of energies of interaction between pairs of atoms and that, in particular,

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Of course, the model [the lattice gas model] is crude, and I can well remember the scepticism with which my own preliminary efforts in the late 1940s to use it as model of liquid-gas equilibrium were greeted. (Domb; 1996, p. 199)

However, as we shall see, Domb did not share the general view on these models.

*interactions between all but nearest neighbour pairs of atoms may be neglected.*  
This can only be a quite crude approximation to the actual configuration energy.(Elcock; 1956, p. 83, emphasis in the original)

So, these assumptions may be crude, but they are not fundamentally wrong. When he compared results for the model obtained in a mean-field approximation, Elcock found some discrepancies between the model and experiments. These can be resolved by solving the Lenz-Ising model without approximations. However, he wrote, other discrepancies remain between the model and experimental data even in an exact treatment of the model. One of them is that it is not justifiable to assume that the energy of configuration can be expressed in terms of interacting pairs.

In his confrontation of the Lenz-Ising model of an alloy with experiments, Elcock tested its assumptions. However, the predictions given by the model were also compared with experiments. In their review article on the theory of alloys, Muto and Takagi (1955) compared the Lenz-Ising model of an alloy with experimental results by C. Sykes and H. Wilkinson from 1937 for the specific heat of  $\beta$  brass. The results for the model were obtained in the mean-field approximation. However, it did not occur to Muto and Takagi that Onsager's solution had shown these approximations to give qualitatively wrong results for the two dimensional model. At any rate, in the mean-field approximation the specific heat of the Lenz-Ising model shows a jump (see section 6.1). Sykes and Wilkinson's results showed that the specific heat is discontinuous rather than infinite at the critical point, so they are in agreement with the predictions yielded by the mean-field approximations. Perhaps this agreement revealed the discrepancy between the approximations and Onsager's solution. Furthermore, they quoted results by Oscar K. Rice purporting to show that Onsager's curve is not exact because the system breaks into two phases of different density. They concluded that "the agreement between theory and experiment is good qualitatively but far from good quantitatively."<sup>23</sup> So, the Lenz-Ising model representing an alloy was perceived as quite realistic and in fair agreement with experiments.

## 7.2 Investigations of the Model in the 1950s

The Lenz-Ising model was the subject of several studies in the 1950s and not only as a representation of alloys. Does this contradict the testimonies described above that the model was perceived as physically irrelevant in the 1950s? In order to answer these questions, it is necessary to look at what the model was used for in these studies. It has already been described that the model as a representation of binary alloys was applied to these phenomena to give insight into them – the predictions of the model were compared with experiments, and the validity of the assumptions of the models was discussed. So, the role of the model within this area will not be dealt with again in the following. Moreover, this section attempts to discuss the opinions about the model generally held in the physics community; consequently, I shall postpone a discussion of the 'dissident' work of Domb and his group to the next section.

I have gone through the papers of the late 1940s and 1950s which according to Science Citation Index cite Ising (1925) and/or Onsager (1944). Most of these papers dealt with technical issues along the lines of Onsager's solution.<sup>24</sup> According to Onsager himself,

<sup>23</sup>Muto and Takagi (1955), p. 245.

<sup>24</sup>They can be classified into the following groups: 1) Attempts at generalisations of Onsager's solution

the model was of interest because mathematical methods available for examining more realistic models were insufficient, and the Lenz-Ising model provides a proof by example that statistical mechanics is capable of accommodating a phase transition. However, he did not think that the model is capable of giving insight into real systems. Are there any reason to believe that the several physicists who found it worthwhile to extend Onsager's work, did think otherwise?

Unfortunately, they rarely placed their work explicitly within a broader context, but simply took the overall goal of examining the model for granted. This means that it is necessary to look at how they actually used the model. Did they confront the model with experiments? Of all the phenomena which the Lenz-Ising model was thought to represent at the time of Onsager's solution, only adsorption of a gas on a surface was a two-dimensional phenomenon. The rest were intrinsically three-dimensional.<sup>25</sup> Both the three-dimensional and two-dimensional model were thought to exhibit singular behaviour but, as already noted by Wannier in 1945, not necessarily of the same nature:

The logarithmic infinity of the specific heat, for instance, is probably due to the fact that the model is two-dimensional. It is not likely to show up in three-dimensional cases. (Wannier; 1945, p. 58)

Consequently, he wrote that the detailed nature of Onsager's result for the twodimensional model was not of as much significance. This means that it only made sense to perform a detailed comparison of Onsager's result on the specific heat with experimental data on adsorption. However, even though experimental results were available for the case of adsorption, such a comparison was not made. In the last part of the 1950s, numerical results concerning the three-dimensional model gradually mounted, thus making a confrontation of the model as a representative of, say, ferromagnetism with experiments possible. However, except for the work of Domb and co-workers (which I shall discuss in section 7.3), nobody published such comparisons. This strengthens the impression that the model was considered to be of little physical relevance.

One gets the feeling that most researchers (again except Domb and his group) were attracted by the mathematical complexity of the problem rather than by the physical application of the model. Indeed, this seems to be supported by a recollection by C. N. Yang of how he got into the work that led to his determination of the spontaneous magnetisation of the two-dimensional Lenz-Ising model. Yang had studied Onsager's solution in 1947, but he first understood the method in 1949 after having consulted Bruria Kaufman's simplified description in Kaufman and Onsager (1949). I believe that my assertion that his driving force was mainly the mathematical problem is evident from the following quotation (the technicalities are not the important thing here):

[...] I did not drop the Ising model. I kept thinking about it, and realised that Onsager and Kaufman had obtained much more information than

to: a) three dimensions, zero magnetic field; and b) two dimensions, but with a magnetic field applied; 2) generalisations of the two dimensional solution to other lattices; 3) attempts at finding exact expressions for quantities of the two-dimensional model not accessible through Onsager's solution, such as the magnetisation and susceptibility. 4) Exact solutions of the three-dimensional model for finite lattices. 5) Finding other solutions than Onsager's for the two-dimensional case which are either simpler or more promising for generalisations to the two-dimensional case. 6) Development of approximative solutions to the three-dimensional model: either by approximating a) the 'mechanism' of the model; or b) the so-called partition function based on series expansions.

<sup>25</sup>The behaviour of two-dimensional ferromagnetic films could be a candidate for a phenomenon represented by the 2D Lenz-Ising model, but its study belongs to a later era.

just the partition function, which was determined by the largest eigenvalue of the transfer matrix. Their method in fact gave information about *all* eigenvalues and eigenvectors. Proceeding in this direction, I arrived in January, 1951, at the conclusion that the spontaneous magnetization is dependent on an off-diagonal matrix element between the *two* eigenvectors with the largest eigenvalues. It seemed to me that, with all the excess information latent in the Onsager-Kaufman method, I should be able to evaluate the matrix element. (Yang; 1983, p. 12, emphasis in the original)

In his recollection, Yang does not put the model into a physical context and repeats the view of the model as a mathematical game discussed on page 94.

The Hungarian-American physicist Laszlo Tisza did in fact put the model to a use outside the mathematical framework. In his proposal of a general theory of phase transitions in 1951,<sup>26</sup> Tisza's main argument against the Ehrenfest classification of phase transitions is that it cannot accommodate the infinities of the Lenz-Ising model. In contrast, Tisza proposed a new, general theory which did not rule out Onsager's results. However, Tisza did not express any opinion as to whether real systems behave like the Lenz-Ising model or not, so it does not seem that Tisza's theory sheds much light on his perception of the model as representation of such systems.

Gregory Wannier had expressed the hope in 1945 that an analytic solution of the three dimensional model might be impending. Onsager himself is said to have worked on a solution to the three-dimensional model around 1956.<sup>27</sup> However, in the 1950s the realization that this solution was not within reach gradually dawned upon physicists. Consequently, the interest in the model waned in the last half of the 1950s, but the model was still well known to, at least, the solid state community (and knowledge of its existence was probably more widespread).

### 7.3 The Motivation and Work of Domb's Group at King's College

One group found the Lenz-Ising model more physically relevant than did the rest of the community, Cyril Domb's. I have already mentioned that Domb has recalled that only a few scientists other than himself were interested in the model in the 1950s. It is worthwhile to examine the motivation behind their work in order to contrast it with the perception of most other physicists. In fact, Michael E. Fisher has written<sup>28</sup> that Domb early understood that simple models are important for an understanding of complex systems, and he cites Domb (1960) as one source in which Domb expressed this view. Indeed Domb wrote here under the heading "simplified models and approximations":

The mathematical problems associated with cooperative assemblies [i. e. systems] are extremely formidable. To facilitate calculations models have been introduced in which the molecular interaction is simplified, but which, it is hoped, maintain the cooperative characteristics of the original assembly; examples are the use of hard sphere molecules in elucidating the properties of

<sup>26</sup>Tisza (1951).

<sup>27</sup>According to Joel Lebowitz, Onsager's post-doc 1956-7. See Lebowitz (1995).

<sup>28</sup>See Fisher (1996).

liquids, and the neglect of all but nearest neighbour interactions in problems on crystal lattices. (Domb; 1960, p. 151)

So, if Fisher is correct and the above quotation is interpreted correctly, Domb seems to be the first who thought that the Lenz-Ising model could give insight into real systems (except, again, for alloys, where this had been known for some time). Consequently, a pertinent question is to examine whether this interpretation is correct. I shall analyse Domb's papers of the 1950s (and the one from 1960 where the above quotation is from). In addition to this examination, the group's work on series expansions, which became of crucial importance in the 1960s, is introduced.

### 7.3.1 Domb's Motivation

I believe that Domb's background is relevant to understanding his motives. At first, Cyril Domb (b. 1920) wanted to pursue a mathematics career and followed the advice of a high school teacher of his that Cambridge University was the place to do so. Consequently, Domb enrolled as a student at this university in 1938 and he passed the Mathematical Tripos (the final exam) in 1941. About his early studies in mathematics, Domb has said:

I never regretted my training as a mathematician. In theoretical physics we are usually pragmatic, and far more concerned with deriving a practical solution to a problem than with establishing rigorously that the solution is correct. But a training in rigour enables one to decide with more confidence when it can be ignored. (Domb; 1990, p. 2)

Even though his education was in mathematics, in Cambridge parlance (applied) mathematics is a broad subject. Several scientists whom others would call theoretical physicists have held chairs in applied mathematics at that university. Moreover, at the Tripos, as Domb has recalled, he "was examined in courses on relativity, quantum mechanics and statistical mechanics, although I attended a variety of additional courses on other topics in pure and applied mathematics."<sup>29</sup> So, Domb received a mathematical training, but with a physical flavour.

After spending the war years on military research, Domb returned to Cambridge in 1946. Here he did his graduate studies in the department of mathematics, which hosted the theoretical physics part of the university:

I had decided that the main area of research for my graduate studies would be statistical mechanics, and Fred Hoyle agreed to serve as my supervisor. He was not actively engaged in research in this area, but I hoped that I would be able to find problems by myself. Fred would let me work on my own and I could discuss my results with him if I felt that I was getting somewhere. (Domb; 1990, p. 9)

The subject of his Ph.D. thesis, which he submitted in 1949, was lattice models of cooperative phenomena.

Domb spent his subsequent professional career, first at the Clarendon Laboratory, Oxford, 1949-52 with a fellowship, then as a lecturer in the mathematics department at Cambridge (which still housed theoretical physics) from 1952-54, and from 1954 as the

<sup>29</sup>Domb (1990), p. 2.



Chair of Theoretical Physics at King's College in London. In 1981 he moved to the Bar-Ilan University in Israel. At King's College he collaborated with Martin Sykes and Michael E. Fisher, among others.

Returning to his work in the 1950s, Domb subscribed to the received view that the model is not a realistic representation of ferromagnets and antiferromagnets, which were his main interest: "Thus although the Ising interaction can only be regarded as a valid approximation for substances exhibiting strong magnetic anisotropy, it has seemed worth analyzing the results in detail, since the statistical aspects of the problem can be most adequately dealt with for this model."<sup>30</sup> In a letter to me,<sup>31</sup> Domb give the following answer to my question of why he chose the Lenz-Ising model rather than the Heisenberg model:

Every physicist concerned with magnetism told us that the Ising model had little physical reality and the proper model to study was the Heisenberg model. But we were concerned with critical behaviour, and it is vastly more difficult to get any information for the Heisenberg model than for the Ising model.

So despite its lack of realism, Domb (and Sykes) found a study of the model worthwhile because its simplicity made it suitable for analysis. The physicists of the 1950s who rejected the Lenz-Ising model, shared the view that the model is simpler than, say, the Heisenberg model, which they preferred. So, Domb agreed with his contemporaries about both the realism and the simplicity of the Lenz-Ising model. Yet he valued the Lenz-Ising model higher than did his contemporary physicists, and he put a substantial amount of efforts into a numerical examination of the model. His interest in the model went back to his graduate studies at Cambridge 1946-1949; the model was the subject of his Ph.D. dissertation of 1949 and of his contribution to the first major conference he attended.<sup>32</sup> Why did Domb have a different view on the value of the model? Either he held a different view on the physical relevance of the model, or he didn't care about its physical relevance but wanted to pursue its mathematical aspects.

If he did care, an explanation for his choice of the model could be his interest in cooperative phenomena in general rather than a specific transition point, say the Curie point of ferromagnets. Already his dissertation dealt with cooperative phenomena in general and he published an article on this subject in 1949 where he discussed binary solutions, ferromagnets, and the order-disorder in solids that "[i]t is clarifying to consider the above problems collectively [...]"<sup>33</sup> Of a correspondingly general nature is the title of Domb and Sykes (1956), 'On Metastable Approximations in Co-operative Assemblies,' while the titles of Domb and Sykes (1957a) and Domb and Sykes (1957b) explicitly refer to ferromagnetism.<sup>34</sup> Since the Lenz-Ising model, in contrast to the Heisenberg model, could represent all these phenomena, it could be used as a starting point for an examination of cooperative phenomena in general. Moreover, in the letter to me referred to above, Domb said about the Lenz-Ising model "[...] that it was very important to show that the same model could apply to different physical phenomena." In sum, his interest in these general phenomena could explain his choice of the Lenz-Ising model.

<sup>30</sup>Domb and Sykes (1957a), p. 216.

<sup>31</sup>Dated March 9, 2005.

<sup>32</sup>Domb (1952).

<sup>33</sup>Domb (1949b), p. 775.

<sup>34</sup>In fact Domb was ten years ahead of his time in this respect: first in the 1960s did others begin to be interested in cooperative phenomena in general rather than in particular phenomena subsumed under this heading.

Another explanation could be that the mathematically trained Domb was more concerned with mathematics than were the rest of the lot. Domb has given the following recollection of how his research started:<sup>35</sup>

My own researches in the statistical mechanics of interacting systems on lattices were sparked off by a colloquium given by A. R. Miller, student of Fowler, on the Bethe approximation and its application to a variety of problems. I realized that for one-dimensional systems I could solve the problem exactly, and this led me naturally to the transfer matrix. (Domb; 1990, p. 12)

His rediscovery of the transfer matrix of Kramers and Wannier, Lassettre and Howe, and Montroll (discussed in Part One) led him to examine the literature: "I was struck by awe and admiration by Onsager's classic 1944 paper".<sup>36</sup> He continues:

I set about formulating transfer matrices for a variety of problems, and I found that they could all be reduced to a simple characteristic form with large numbers of zeros, which I called *duo-diagonal*. At this period I hoped that it would be possible to deal with these matrices exactly, and I consulted with Philip Hall; but he was convinced that the problem was very difficult and had no practical suggestions to offer. I therefore developed perturbation expansions for the two-dimensional Ising model in zero and non-zero field. (Domb; 1990, p. 12, emphasis in the original)

So, based on these remarks, his motivation is judged to be of a mathematical nature rather than grounded in physical relevance: Domb had a *method*, the transfer matrix, and looked for problems to solve, rather than for methods to solve a pertinent problem.

The assumption that Domb himself considered his work very mathematical is corroborated by an unpublished correspondence with Rudolf Peierls. In 1947, Domb sent a manuscript on "Order-Disorder Statistics" through his supervisor Fred Hoyle to Peierls. In one of the subsequent letters, Domb wrote "I realise that my approach is very mathematical, and that there is therefore a danger of not concentrating on the physical[ly] important features."<sup>37</sup>

As I shall document below, Domb's hard work on series expansions gave him several opportunities for confrontation of the model with experiments, but only in one case did he actually do so. I take this as evidence that he was mainly occupied with the mathematical problems related to the model rather than its direct relevance to real systems.

### 7.3.2 Series Expansions

In the late 1940s and in the 1950s, the set of exact results on the two dimensional Lenz-Ising model was extended, most importantly by Yang's result on the magnetisation and by others' generalisations of Onsager's results to other types of lattices. The three-dimensional variant, on the other hand, resisted attacks of getting an exact solution. However, in the 1950s the three-dimensional model was examined by applying series expansions and even though the results thus obtained were inexact, as well as based on

<sup>35</sup>His recollections in a interview with the Physics of Scale group are essentially identical to the quotation.

<sup>36</sup>Domb (1990), p. 12.

<sup>37</sup>Letter from C. Domb to R. E. Peierls, October 14, 1947. In the Bodleian Library, Oxford, C72, MS Eng. Misc, b 205.

new assumptions (whose validity could not be rigorously checked), information about the critical behaviour of the model, which was thought to be reliable, could be obtained. Consequently, a comparison of the three-dimensional model with experiments became possible.

Domb was the first to advance the idea of correlating the coefficients of lengthy series expansions with critical behaviour, which he did in his doctoral dissertation of 1949, and he was soon followed by others, mainly Rushbrooke and his group of the University of Newcastle.<sup>38</sup> The method of high and low temperature series expansions had been applied to models since the 1930s. For instance, Kramers and Wannier had used the work of others to assess various closed-form approximation in their papers of 1941. Moreover, series expansions were used in the 1950s, for instance by Freeman Dyson in a work on the Heisenberg model.<sup>39</sup> However, the approach of Domb, Rushbrooke and their groups distinguished itself from the previous ones because it was more systematic, contained more terms than the previous ones and the terms obtained were exact.<sup>40</sup>

The general method was to obtain a series from a perturbation expansion, typically of the free energy. The coefficients of the series were then correlated with the critical behaviour by means of a guess of the singularity at the critical point. Even though the number of terms was large, it was finite and this gave a fundamental problem:

Now any second-year mathematics student will tell you that nothing can be learned about the singularities of a function from a finite number of terms of a series expansions; for example, even if the first 15 terms of an expansion are positive and well-behaved, there is nothing to ensure that an effect which is small and unnoticed in the first few terms will not dominate asymptotically [...], but the following physical considerations enable one, nevertheless, in many cases, to make confident predictions about the singularities of functions from a finite number of terms of series expansions.

(a) The two-dimensional solution can act as a guide since we expect the three-dimensional solution to be similar to it in essential features.

(b) We have a few exact theorems which apply to three-dimensional solutions.

(c) Physical considerations of what is expected of the model can lead us to transformations of the series which reveal peculiarities of behaviour. (Domb; 1966, p. 29)

Series expansions allowed physicists to obtain approximately the critical behaviour of the Lenz-Ising model in two and three dimensions and also for non-zero fields. In the wake of Onsager's solution a number of exact results on the two dimensional model appeared which could be confronted with results of series expansions, and the agreement was generally found to be good. So, in 1960 Domb could write:

<sup>38</sup>Domb (1996), pp. 148-9.

<sup>39</sup>Domb has written about Dyson's paper:

For the Heisenberg model the density and low-temperature expansions are related to the interaction of spin waves, a difficult problem first tackled effectively by Dyson (1956); but the number of terms he calculated are insufficient to throw any light on critical behaviour. (Domb; 1996, p. 7)

<sup>40</sup>Hoddeson, Shubert, Heims and Baym (1992).

By combining information from series expansions and higher order approximations in closed form, we believe that most of the important properties of the three-dimensional model can be *reliably* established [...]. We should then be in a better position to compare the results with experiment, and to see whether a serious refinement of the model is needed to secure effective agreement. (Domb; 1960, p. 246, my emphasis)

The expansions were mainly used for ferromagnets and antiferromagnets. Rushbrooke and co-workers applied such expansions to the Heisenberg model, but Domb and his group were the only ones who obtained results concerning the critical behaviour of the Lenz-Ising model. Extensive efforts were put into handling these expansions, because not only every dimension, but also every type of lattice demanded a separate calculation, but within a few years reliable information about the critical behaviour of a number of cases was obtained. Not everybody found the series expansions worthwhile. To quote Domb:

Some people have no enthusiasm for methods which are not exact and consider that detailed investigation of higher order approximation terms is not the task of a theoretical physicist. I am reminded of a conversation which I had with [Jacques] Yvon about his own important contribution to this field [...]. He told me that he had developed the method, tried it in lower order, and found that it gave the same result as other approximations. I asked if he had not been interested to go to higher orders to see whether it gave any improvement. He replied: 'my task as a theoretical physicist is to develop methods, and see that they work and are correct; I then hand over to engineers.' (Domb; 1966, p. 29)

### 7.3.3 Comparisons with Experiments

Turning now to the use of these numerical results, Domb and co-workers compared the Lenz-Ising ferromagnet with experimental results in the 1950s. Domb related the model to experiments for the first time at the Paris Conference in 1952 on changes of phases. In an account of the similarities between the two dimensional model on different lattices, he noted a discrepancy between this model and experimental results:<sup>41</sup>

Thus the specific heat [of the two-dimensional model] is logarithmic infinite on both sides of the Curie point, and differs considerably from any experimentally observed specific heat curves. Perhaps the most marked difference

<sup>41</sup>Four years later, Domb and Sykes (1956) gave the same statement, this time in English where the translation of the French text in Domb (1952) is taken from. The French text reads:

Ainsi la chaleur spécifique tend logarithmiquement vers l'infini des deux côtés du point Curie et diffère considérablement des courbes expérimentales de chaleur spécifique.

La différence la plus frappante est peut-être la longue 'queue' dans les courbes théoriques de chaleurs spécifiques, qui indique qu'une fraction importante du changement d'entropie totale du système a lieu dans le domaine de température situé au-dessus du point de Curie. (Domb; 1952, p. 192)

In fact, Domb stuck to this statement another four years later where he wrote: "The specific heat of the three-dimensional model seems to remain infinite at the Curie point, but its detailed shape is appreciably different from the Onsager curve in two dimensions. The 'tail' is far smaller, showing that most of the entropy change of the assembly takes place in the temperature region below the Curie point; this is in far better agreement with experimental observations of specific heat anomalies." (Domb; 1960, p. 286).

is the large ‘tail’ of the theoretical specific heat curve, which shows that a substantial fraction of the total entropy change of the system takes place in the temperature region above the Curie point. (Domb; 1952, p. 192)

Domb neither specified his source of the experiments which revealed this discrepancy,<sup>42</sup> nor did he provide a comparison of the curves. In fact, the main role of mentioning the discrepancy was to justify the examination of the three-dimensional variant of the Lenz-Ising model: “It is of great interest, therefore, to determine how these features are modified when a more realistic three-dimensional model is used.”<sup>43</sup>

The use of series expansions allowed Domb to obtain the specific heat  $c_v$  as a function of temperature for the three-dimensional Lenz-Ising model, but these results, too, were not confronted with experimental curves. Rather, he examined the “difference between specific heat curves for various lattices [...]”,<sup>44</sup> from which he concluded that the ‘tail’ of the specific heat of three-dimensional models on various lattices is reduced compared to their two-dimensional counterparts. Consequently, for the former models “this must lead to a specific heat curve in closer agreement with experimental curves.” Considering the very few confrontations of the model with experiments, I believe it is fair to say that Domb’s purpose was not a test of the model by means of experiments.

Domb continued this work in a series of three papers,<sup>45</sup> with his former graduate student from Oxford, Martin F. Sykes. They not only obtained specific heat results for other lattices, but also applied the series expansion method to the susceptibility of the Lenz-Ising ferromagnet. However, the overall picture is the same as above: they almost refrained from confronting their results with experimental results. Based on their numerical results, Domb (1960) drew in his review paper a curve for the specific heat from  $T/T_c = 0$  to  $T/T_c = 2$ , but he did still not confront it with experimental results. So, the comparison of this quantity with experimental results was not the main focus of Domb and Sykes. Rather it was the similarities and differences between the model ‘living’ on different lattices.

Domb and Sykes did actually publish one paper<sup>46</sup> which contained a section on the relation between experiments and model predictions. Here they compared the experimental results for nickel by Weiss and Forrer from the end of the 1920s<sup>47</sup> with high temperature expansions, even though nickel does not have the strong magnetic anisotropy of the Lenz-Ising interaction. Domb and Sykes plotted the inverse zero field susceptibility calculated for the face-centred cubic Ising model with spin  $\frac{1}{2}$  together with experimental values:

The two curves have been made to coincide at  $T/T_c = 1.2$  by multiplying the values quoted by Néel by  $5.36 \times 10^{-6}$ . On the scale adopted agreement is

<sup>42</sup>Perhaps because he considered it to be common knowledge? A possible source for this knowledge could be C. Sykes and H. Wilkinson’s review of experiments on the specific heat of nickel. See Sykes and Wilkinson (1938).

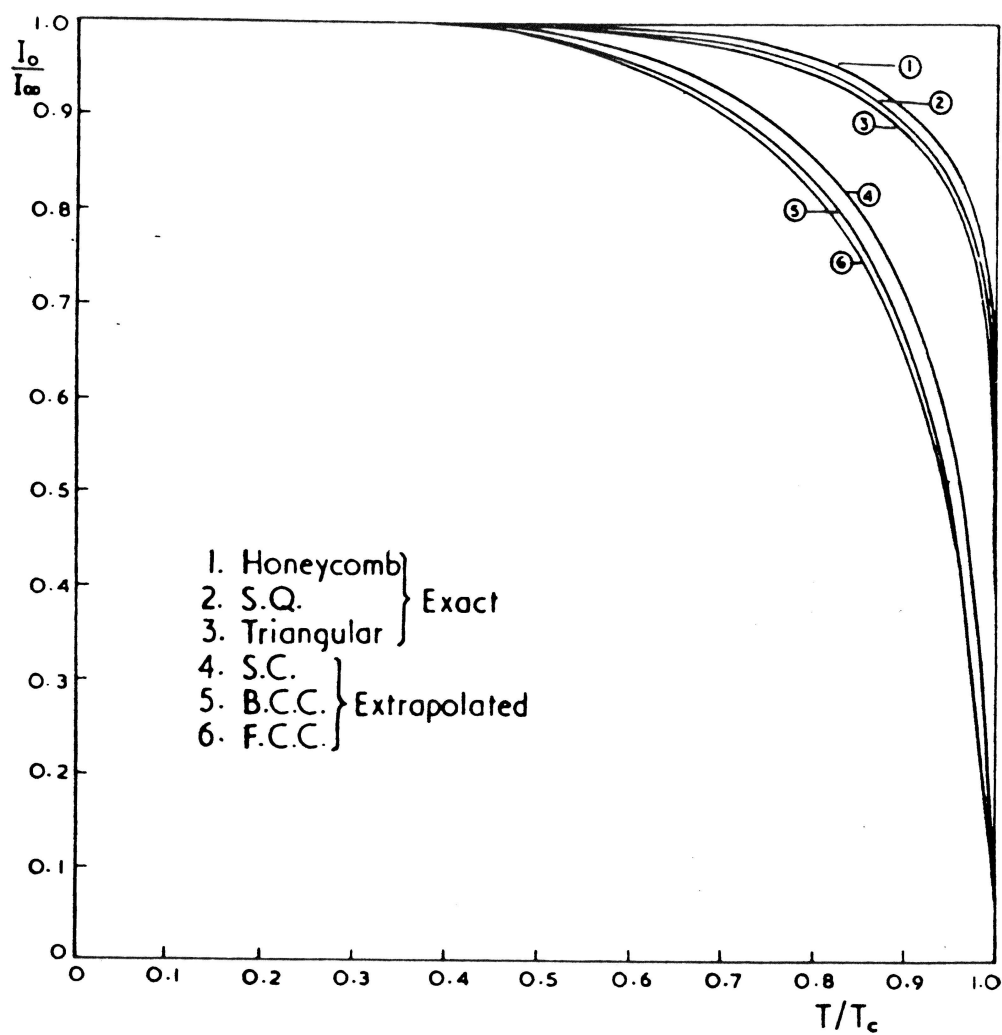
<sup>43</sup>Domb (1952), p. 192. The French text reads “Il est donc très intéressant de déterminer comment cet aspect se trouve modifié si on utilise un modèle tridimensionnel plus proche de la réalité.”

<sup>44</sup>Domb (1952), p. 195. The French text reads: “les différences entre les courbes des chaleur spécifique pour différents réseaux[...]”.

<sup>45</sup>Domb and Sykes (1956), Domb and Sykes (1957a), and Domb and Sykes (1957b). The first is by and large identical to Domb (1952) as far as the physical contents are concerned (they have the same sentences about physical relevance and quantities of interest to compare). The difference seems to be that the article with Sykes are based on longer expansions.

<sup>46</sup>Domb and Sykes (1957a).

<sup>47</sup>Incidentally these results were quite popular: They were used in 1934 by Néel and later by Kouvel and Fisher (1964).



**Figure 7.1:** The spontaneous magnetisation for the Lenz-Ising model. From Burley (1960).

complete in the curved region below  $T/T_c = 1.2$ , the discrepancies being not greater than 2% except in the very small region 0 to 3% above the Curie point where the shape of the theoretical curve is most sensitive to small changes in the extrapolated values of  $T_c$  and  $h$  and the shape of the experimental curve is most sensitive to the experimental value of the Curie adopted. To draw figure 5 we have taken the experimental Curie temperature as  $629^\circ \text{A}$  [sic, they probably meant K], this value being obtained by extrapolating the inverse susceptibility to zero. (Domb and Sykes; 1957a, p. 227)

This made them conclude in the abstract: “The experimental curve of Weiss & Forrer for nickel is examined, and it is found that the data can be fitted quite well by the extrapolation formula for a three-dimensional lattice.” (Domb and Sykes; 1957a, p. 214)

This is the only example where they thoroughly confronted the model with experiments. That others refrained from comparisons, is illustrated by a paper by D. M. Burley at the brink of the decade, based on his dissertation of 1960 from the University of London.<sup>48</sup> He applied the series expansion method of Domb and Sykes (1956) to the low temperature spontaneous magnetisation for the three dimensional Lenz-Ising model on three lattices, simple cubic (sc), body-centred cubic (bcc), and face-centred cubic (fcc), and determined the curve for the magnetisation given in figure 7.1. However, neither he nor Domb, who quoted Burley’s results in Domb (1960), compared the obtained curves with experimental results. Instead, Burley wrote:

Since the Ising model treats spin as a classical property, quantitative agreement with experiment is not to be expected, but despite the considerable idealization of the model good qualitative agreement is obtained, the spontaneous magnetization curves going to zero at the critical temperature. The importance of the quantum nature of spin is shown well by the better quantitative agreement obtained at low temperatures from the spin wave treatment of the Heisenberg model (Dyson, 1956). (Burley; 1960, p. 912)

Returning to Domb, from these results he concluded:

Thus we find again that the dimension of a model is the major factor in determining the shape of the spontaneous magnetization curve, the difference in crystal lattice leading only to a ‘fine structure’ variation. (Domb; 1960, p. 293)

So, on the one hand Domb wrote that the three-dimensional model is more realistic, but on the other hand he did not compare it with experimental results. This is remarkable in view of the efforts he had put into obtaining these theoretical results. Why not see whether the model is in agreement with real systems? Domb (1960) did examine the validity of various approximative methods. So, it is natural to conclude that for Domb at this time, the examination of approximative methods was much more important than the confrontation of the model with experiments.

Since there was only a comparison in one of Domb and Sykes’s papers, despite the possibility of making one in a number of other cases, we must conclude that they did not show much interest in such confrontations. This is even more remarkable considering the fact that Domb (1960) wrote that series expansions had reached a state where “if

<sup>48</sup>Burley published some of his result in Burley (1960), which is the basis of the following discussion.

there is disagreement with experimental results [and the Lenz-Ising model],”<sup>49</sup> it could be concluded that this must be due to inadequacy of the model, rather than to the approximation. However, he did not at all make a systematic comparison of the model with experiments. Returning to the question of Domb’s motivation I am inclined to think that his mathematical training rather than his interest in cooperative phenomena made him particularly interested in the Lenz-Ising model. Moreover, on this basis, I find it hard to defend the view that he was the first to think that simple models in general and the Lenz-Ising model in particular would give understanding of real systems as asserted by Fisher above.

That Burley found the model incapable of giving direct insight into real systems is revealed by the following statement. After having dismissed the Lenz-Ising model due to its classical spin, Burley wrote:

This work on the Ising model is important, nevertheless, on two counts. Firstly, the data obtained give a valuable yardstick by which more physically realistic models and approximate methods, used for the models, can be measured. Secondly, fig. 1 [figure 7.1 here] shows clearly that the dimensionality of the lattice is the most important feature to be considered and that the co-ordination number of the lattice only affects the fine structure of the curves. (Burley; 1960, p. 912)

This second reason must be that since Burley’s results reveal the strong dependence on dimensionality of the Lenz-Ising model, this might also be the case for more realistic models. I believe that Domb and the members of his group would subscribe to Burley’s view.

According to this view the models are not interesting in themselves but because of the light they shed on other models. As we shall see, physicists of the 1960s thought that the Lenz-Ising model was relevant in itself. So, in this crucial respect, Burley differs from the attitude of the 1960s physicists.

## 7.4 Summary

To conclude, the following assessment about the perception of the Lenz-Ising model in the 1950s can be made. Only a small number of scientists studied the model in this decade, and those who did were mainly motivated by it as a mathematical game and they did not compare the model with experiments. This attitude, that the model was mathematically interesting but physically irrelevant, is reflected in both contemporary and retrospective statements. So, it seems fair to conclude that the general attitude towards the model was that it is not relevant to use the model to obtain insight into real physical systems. Most physicists preferred the Heisenberg model to the Lenz-Ising model when it comes to ferromagnetism and we shall see later that they preferred Mayer’s model in the area of liquid-gas phenomena. The Lenz-Ising model was a well-known model in the 1950s, so this must have been a conscious choice.

However, one group, Domb’s at King’s College, London, seems to have held another attitude towards the model. Domb and co-workers did compare the model with experimental results, but to so small an extent that it is difficult to conclude that they found the model of much relevance to real systems. Rather, they seem to have studied the model

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<sup>49</sup>Domb (1960), p. 152.



in order to learn about other models. However, their studies played an important role because when the model later was found relevant the results of the group proved useful.

One strategy, which a modern physicist probably would find natural or even self-evident, is to start by examining the most simple model, even if it is only known to be slightly related to the phenomenon, to see to what extent this model agrees with experiments. First then would one throw oneself into more realistic, but also more complicated model. As shown above this strategy was only used by a handful of physicists in the 1950s, most notably Domb and his group. They started with the Lenz-Ising model to see how far that examinations of the model would lead. The majority of physicists chose to start with the more realistic models, mainly the Heisenberg model. Once again, this must have been a conscious choice.

# 8

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## From Irrelevance to Relevance

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In the 1960s things changed. The perception of the physical relevance of the Lenz-Ising model changed – the model went from being seen as a toy model capable of showing the possibility of phase transitions to a caricature model revealing (some of) the actual physics that the model was built to represent. In Chapters 10 and 11 I examine how the model was put to a use during the 1960s. The main point will be that a change occurred in this respect: in the first part of the 1960s, the model was used to give insight into real systems, but it was mainly applied to solve specific tasks. In the last half of that decade, however, the model formed the basis of a more general and systematic account of critical phenomena. I am principally interested in understanding why the model was found capable of doing the latter job. However, in order to do so it is necessary to understand the same question for the first half of the decade. It was during those years that the model was first perceived to provide insight into real systems.

So, the present chapter seeks an answer to the following question: Why was the model ‘all of a sudden’ perceived in the first half of the 1960s as giving physical insight? I shall argue that this change in the perception of the model was not due to a change in the perception of the realism of the model, but to the realisation that the model agrees with certain experiments.

In the first part of the 1960s information accumulated on two fronts. On the one hand, experimental results concerning the critical region had been obtained. Since 1961, experimental data mounted on the equilibrium properties of a host of magnetic materials.<sup>1</sup> Furthermore, old results were being revisited in light of new theoretical developments. The tradition in the area of liquid-gas critical points went back several years, but also received new attention in the 1960s.<sup>2</sup> On the other hand, the use of series expansions continued and provided a host of numerical results on the critical behaviour of the Lenz-Ising model and, to a lesser extent, the Heisenberg model. In particular, George A. Baker’s introduction of Padé Approximants (1961) into the field of series expansions was a crucial event, because it considerably extended the set of singularities which could be studied by the series expansions.<sup>3</sup>

In order to assess the perception of the Lenz-Ising model in the 1960s, its theoretical and experimental status is reviewed.

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<sup>1</sup>Benedek (1966).

<sup>2</sup>Domb (1996).

<sup>3</sup>In contrast to previous methods, Padé Approximants could tackle series with alternating signs. See Domb (1996), pp. 165-166.

## 8.1 Theoretical Status of Models

In his lectures on critical phenomena delivered at the Summer Institute for Theoretical Physics at University of Colorado, Boulder, in 1964,<sup>4</sup> Michael E. Fisher presented several of the models in play in the area of critical phenomena. Here, Fisher explicitly stated his attitude towards the realism of the models, so the lecture notes can be used to assess the perception of models discussed. In view of the educational purpose of the lectures, they probably reflect a sort of consensus view of the models at the time.

Fisher began his lectures at Boulder by subscribing to the Russian physicist Yakov I. Frenkel's view on the task of the theoretical physicist: "The first task, recalling Frenkel's advice, is to construct some simple physical models on which to base our theoretical calculations."<sup>5</sup> I have much more to say about Fisher's modelling approach later on; here his presentation of five models is in focus. His treatment of these models, which includes the Lenz-Ising model, but also more realistic models, reveals that by and large he shared the views of the realism of these models held by most physicists of the 1950s. It seems well advised to go through Fisher's treatment in more detail than simply noting his agreement with his colleagues of the previous decade. The first reason for this is that the treatment documents his, and probably many other's, attitude towards simple models in the 1960s. He ranks the models according to their realism, evincing in a very clear manner his perception of how the models are placed with respect to each other. In other words, Fisher's quite detailed characterisation of models gives an important snapshot of the views of models around 1964. The second reason is for future reference: A few years later Fisher was the main proponent of a new view of the use of models (which will be treated in Chapter 11) and his 1964 treatment is a valuable source of information about his views.

Fisher divided the models into 'simple' and 'simpler' according to what I have termed the realism of models, in Chapter 2. The empirical adequacy of a model has nothing to do with its realism. Under the heading 'simple models', Fisher talked about a) the classical continuum gas; b) the Heisenberg model for magnetism; c) binary alloys. He wrote concerning the realism of these models: "Of the three models discussed, the classical continuum gas model is probably the most realistic."<sup>6</sup>

The development of the classical continuum gas model will be treated in detail in Chapter 9, so here it suffices to introduce its three assumptions, which are that the atoms or molecules of the gas interact pairwise and via central forces and that classical mechanics, rather than quantum mechanics, should apply to the system. Fisher wrote about this model that it "[...] is so familiar that the theorist is apt to forget that it is *only a model* of real physical systems."<sup>7</sup>

This high degree of confidence in this model was based on the possibility of giving credence to the three underlying assumptions. This is reflected in his discussion of their validity. About the use of classical mechanics he wrote that it "seems quite justifiable for most gases near their critical temperatures."<sup>8</sup> He said that only for hydrogen, helium, and maybe neon, should one have serious reservations. Concerning pairwise forces, quantum mechanical treatments of many-body forces between atoms or molecules reveal that

<sup>4</sup>Published in the following year as Fisher (1965).

<sup>5</sup>Fisher (1965), p. 24.

<sup>6</sup>Fisher (1965), p. 27.

<sup>7</sup>Fisher (1965), p. 24, Emphasis in original.

<sup>8</sup>Fisher (1965), p. 24.

the assumption of pairwise forces is “not entirely correct.”<sup>9</sup> However, he continued, “except at high densities the three-body and higher order forces are numerically small and it seems safe to neglect them near critical densities [...] in a first discussion.”<sup>10</sup> For monatomic gases the assumption of central forces, i.e., that the potential  $\phi$  can be written as a function of the distance  $r$  rather than the vector  $\mathbf{r}$ , is “good”.<sup>11</sup> However, it is probably “less accurate”<sup>12</sup> for non-symmetric molecules, e.g., diatomic ones.

These are the three fundamental assumptions about the classical gas. However, more assumptions about the form of the pair potential are required. Fisher wrote: “One knows, of course, that the correct pair potential,  $\phi(r)$ , should have a strongly repulsive core followed by a relatively weak attractive well and an attractive tail decaying as  $1/r^6$ .”<sup>13</sup> What I have termed the Mayer model in the next chapter is obtained if a further assumption is added, namely that the potential is of finite range  $b$ , i.e.,  $\phi(r) \equiv 0$  for  $r > b$ . Fisher wrote about this further assumption that “one feels that this should not matter too seriously.”<sup>14</sup>

Turning to the (general) Heisenberg model, it rests on three fundamental assumptions: i) localised spins; ii) pairwise interaction; and iii) complete isotropy so that the Hamiltonian is invariant under rotation of the total spin. Concerning the second assumption, Fisher only remarked that it “seems reasonable on a first approach”<sup>15</sup>, but he had more to say about the other two. The first assumption says that it is possible to associate a spin variable  $\vec{S}_i$  to site  $i$ . Fisher shared van Vleck’s criticism of localised spins expressed on page 95, but discussed its domain of validity:

This should be justifiable for insulation crystals but is certainly open to question for good conductors such as iron and nickel. Indeed in the latter case the zero temperature saturation moment indicates that only 0.6 of the usual electronic magnetic moment is available per ion. (Fisher; 1965, p. 25).

Concerning assumption three, Fisher wrote that all real magnets exhibit some degree of anisotropy and even a small anisotropy can help stabilising the direction of magnetisation. He then devised a way in which this anisotropy can be taken into account by modifying the Heisenberg Hamiltonian, but “in many cases we may hope to avoid these refinements”.<sup>16</sup>

These three assumptions lead to a general Heisenberg Hamiltonian for  $N$  ions:

$$\mathcal{H} = - \sum_{i=1}^N \sum_{j=1}^N J_{ij} \vec{S}_i \cdot \vec{S}_j - g\beta_B \sum_{i=1}^N \vec{S}_i \cdot \vec{H} \quad (8.1)$$

where  $\vec{H}$  is the magnetic field,  $g\beta_B$  is essentially the magnetic moment per spin and  $J_{ij}$  is the exchange energy between spins  $i$  and  $j$ .

Fisher then introduced a fourth assumptions, that of restricting interactions to nearest neighbour pairs with the same exchange constant  $J$ . He justified this assumption in the following way:

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<sup>9</sup>Fisher (1965), p. 24.

<sup>10</sup>Fisher (1965), p. 24-25.

<sup>11</sup>Fisher (1965), p. 25.

<sup>12</sup>Fisher (1965), p. 25.

<sup>13</sup>Fisher (1965), p. 25.

<sup>14</sup>Fisher (1965), p. 25.

<sup>15</sup>Fisher (1965), p. 25.

<sup>16</sup>Fisher (1965), p. 26.

Although there is ample evidence to show that second and further neighbour interactions are *not* in general negligible they should not matter crucially if they do not oppose the ordering tendencies of the dominant first neighbour interactions. Conversely, when this is *not* true one sees the more complicated magnetic behaviour which we have elected not to discuss. (Fisher; 1965, p. 26, emphasis in the original)

The “last ‘fairly realistic’ simple model” is almost equivalent to the Lenz-Ising model for binary alloys of A and B atoms, but Fisher allowed the interaction energy between two atoms of the same kind to cost different energies. The assumptions of this model imply, he wrote,

the neglect of any interactions with the lattice vibrations. This cannot be very accurate since if the masses  $m_A$  and  $m_B$  are distinct even the zero point lattice energy will depend on the degree of order. (Fisher; 1965, p. 26)

On the other hand, he continued, if the interaction energies are not rapidly varying with lattice spacing and the masses of the two types of atoms are not very different, the effect of the lattice vibrations would probably only be a “renormalization”<sup>17</sup> of the energies. It is not quite clear to me what he meant by this, but it could be that the energy scale but not their mutual magnitudes is changed by the lattice vibrations. The assumptions also ignore the role of unequal atomic sizes of the two types of ions “which might well be important if these differ appreciably.”<sup>18</sup> Despite all these shortcomings, he concluded that “Nevertheless, one feels that the model ought to yield a fairly reliable description of the ordering phenomenon.”<sup>19</sup>

Fisher did not explicitly describe the characteristics of a ‘simple model’. However, it is possible to extract the following implicit description from his examples. A simple model is based on assumptions which are not strictly true and in fact introduce abstractions and idealisations which are known to be incorrect. While the effect of these simplifications are non-negligible, it is often possible to argue that they are not of crucial importance. At least there are several particular cases where this is true, for instance insulation crystals of ferromagnetism where the assumption of well-localised spins for the Heisenberg model is thought to be reasonable, which is not the case for good conductors. Fisher can therefore characterise simple models as “fairly realistic” and yielding a “fairly reliable description.”

After ‘simple models,’ Fisher turned to ‘simpler models,’ that is the lattice gas model and the magnetic Lenz-Ising model. Both models were introduced as approximations to the previous models. For the lattice gas model he started with the assumptions that the molecules live on the sites of a lattice of spacing  $\delta$ . This assumption, he wrote, corresponds to replacing integrals in the partition function with approximating Riemann sums. “Consequently, if the lattice spacing  $\delta$  is small compared with the distances over which the pair potential varies appreciably, any errors should be negligible except perhaps at densities near close-packing.”<sup>20</sup> On the other hand, at high densities where the particles are close to each other, the precise distance between two particles becomes important, so the model has “some artificial features” and does not yield the correct behaviour for high densities, so close qualitative agreement with real gases is not to be expected. “However,”

<sup>17</sup>Fisher (1965), p. 26.

<sup>18</sup>Fisher (1965), p. 26.

<sup>19</sup>Fisher (1965), p. 26.

<sup>20</sup>Fisher (1965), p. 27.

he continued, "the model, [...] still contains the 'seeds of reality' and it transpires that it yields a surprisingly accurate account of the critical point phenomena."<sup>21</sup>

He then turned to the Lenz-Ising model for magnetism which was also justified by appeal to the mathematical problems of the more realistic model:

Finally, let us simplify the Heisenberg model. Although in many ways this is not as intractable as the continuum gas model (thus the low temperature properties may be described accurately, even though only asymptotically, in terms of spin waves and progress can also be made at high temperatures), the noncommutation of the operators makes extensive calculation difficult. (Fisher; 1965, p. 27-8).

The simplification led to the Lenz-Ising model:

One of the most artificial aspects of the Ising model interaction is its extreme anisotropy which results, in particular, in an essentially complete absence of spin waves behaviour at low temperatures. However, our interests will be at high temperatures close to the critical point where this deficiency can be expected to be less significant (and where the concept of a spin wave loses its validity). (Fisher; 1965, p. 28).

Furthermore, Fisher used the discovery of 'Ising-like' magnetic crystals (e.g., the antiferromagnet dysprosium aluminium garnet) to justify the model. However, even though such exotic materials have been found, they constitute only a small fraction of the relevant materials, and the conceptually most important materials are not included in this category.

From Fisher's examples it is clear that the models in the category 'simpler models' are characterised by the fact that one (or more) of the assumptions is (are) perceived as very problematic and often incorrect, at least in some limit (for instance, the high density limit). Thus the assumption makes the model 'artificial.' While the range of validity of a simple model is subject to control, this is not the case for the problematic assumption of a 'simpler model.' However, a simple model can still contain the 'seeds of reality.'

To sum up, Fisher presented the following – probably widespread – view on the models: for ferromagnets and antiferromagnets, the Heisenberg model was on a much more theoretically secure footing than the Lenz-Ising model. The classical continuum gas model was more realistic than the lattice gas model as a representation of gases. However, the Lenz-Ising alloy model was the most realistic model available for these phenomena. This ranking is reflected in Fisher's classification of the models: While he put the Lenz-Ising model as a representation of a binary alloy in the category 'simple models,' the model as a lattice gas, a representation of a ferromagnet or an antiferromagnet belonged to the category 'simpler models.' So, the consensus view on the realism of these models circa 1964 was the same as that of the 1940s and 1950s.

## 8.2 The Experimental Situation

What about the experimental situation? In the 1960s the Lenz-Ising model was confronted with experimental results, first and foremost the lattice gas model. It was found that the model does have some empirical adequacy. This section traces the development which led to this recognition.

<sup>21</sup>Fisher (1965), p. 27.

Experiments on critical behaviour are exceedingly difficult to perform. It is beyond the scope of the dissertation to treat the advances in experimental methods which led to accurate measurement in neighbourhood of the critical point. I shall only rely on the assessments of experiments by contemporary, mainly theoretical physicists.

### 8.2.1 Binary alloys

As noted in Chapter 7, three-dimensional Lenz-Ising alloys were in fact compared with experiments. Since the method of series expansions had not diffused into this area, mean-field approximative methods were used instead to examine the model. This means that experiments were confronted with model result based on approximations known by physicists (at least in the area of magnetism) to introduce spurious effects for the two-dimensional case.<sup>22</sup> Ironically, the experiments used for the specific heat,<sup>23</sup> showed a discontinuity in this important quantity, in contrast to Onsager's solution but in agreement with solutions obtained by approximative methods. Consequently, the invalidity of the latter methods seems to have received no attention. So, in this area – the one which the Lenz-Ising model was generally found to be most realistically representing – the model (without the invalid methods) was in fact not confronted with experiments prior to the 1960s.

### 8.2.2 Superfluid Helium

The first area in which experimental results emerged which seemed to have features in common with the Lenz-Ising model was the area of superfluid helium and its lambda transition point from the normal liquid state to the super fluid one.

One of the first hints that there might be agreement between the model and experiments was the fact that both the Lenz-Ising model and liquid helium show an infinite singularity in the specific heat. That this is the case for liquid helium was first suggested by Lazlo Tisza in 1951,<sup>24</sup> but it did not seem to be an accepted fact.<sup>25</sup> Tisza also observed that Onsager's solution yields a singularity, but he did not ascribe too much significance to the logarithmic nature of the specific heat because of its origin in the *two*-dimensional model. The fact that liquid helium and the Onsager solution both yield an infinite singularity may not sound as much of an agreement between the model and experiment, but in a situation where the Onsager solution was mainly perceived as merely a mathematical curiosity, even such small agreements might have given some physical credence to the Lenz-Ising model.

In 1959 Fairbank, Buckingham, and Kellers pointed out that there is agreement between the model and experiments.<sup>26</sup> Two years later, Buckingham and Fairbank coupled

<sup>22</sup>At least this was the case in Muto and Takagi (1955) and Wojtowicz and Kirkwood (1960).

<sup>23</sup>Obtained by C. Sykes and H. Wilkinson in 1937.

<sup>24</sup>Buckingham and Fairbank (1961).

<sup>25</sup>Buckingham and Fairbank (1961) wrote that Blatt, Butler, Schafroth as late as 1956 suggested that the specific heat has a maximum rather than an infinity.

<sup>26</sup>Buckingham and Fairbank (1961). In 1954, Atkins and Edwards published measurements of the coefficient of expansion for liquid helium in the vicinity of the  $\lambda$  point and found that below the  $\lambda$  point, this quantity is logarithmic in  $T_\lambda - T$ . As an aside, they wrote that this is "of particular interest because Onsager [...] has discussed a two-dimensional model of a ferromagnetic and has shown that the specific heat in the vicinity of the Curie point is  $C_p = A \log(T_c - T) + B$ ." (Atkins and Edwards; 1955, p. 1433). However, this conclusion does not seem to have had much impact, probably due to the fact that there is not direct connection

this result to the “notoriously difficult”<sup>27</sup> problem of a statistical theory of cooperative phenomena and Onsager’s solution with the words:

It is a striking fact that the nature of the singularity with this exact solution is of just the same form as that observed in the liquid helium transition. It may well prove to be the case that this particular form is characteristic of cooperative transitions, in spite of the fact that there are, in principle, many possibilities available. (Buckingham and Fairbank; 1961, p. 81)

This seems to be the first statement that the Lenz-Ising model is empirically adequate.<sup>28</sup> They were vague about the conclusions to be drawn from this adequacy of the model. At any rate, this was the first time that someone opened for the possibility that the model might capture some essential features of cooperative transitions.

There was, however, one problem for scientists interested in critical phenomena. This was stated by Michael E. Fisher: “The behaviour of helium, however, is presumably determined essentially by quantum mechanics and it is not clear how far one should expect an analogy with the ‘classical’ critical points.”<sup>29</sup> As Fisher’s (and most others) main interest was classical critical points, he only mentioned the results by Buckingham and Fairbank in a footnote and concentrated on xenon and argon. This reflects a general attitude that liquid helium did not have much to say about classical critical points. This objection seems to have had a rub-off effect on the perception of the importance of the adequacy of the model; the model was not perceived as a good representation of liquid helium.

### 8.2.3 Gas-Liquid Transition

The critical points of xenon, argon and oxygen do not suffer from this deficiency and the investigation of these points played a crucial role for changing the perception of the model. A group at the National Research Council Laboratories in Ottawa, Canada, which included H. W. Habgood, W. G. Schneider and M. A. Weinberger, had the measurement of a number of properties of xenon in the critical region as a programme in the 1950s. I shall be concerned only with the liquid vapour coexistence curve and the compressibility.<sup>30</sup> Xenon was chosen because it is monatomic and has a critical temperature close to room temperature.<sup>31</sup> The first to compare the results of this group with the Lenz-Ising model (i.e., in the lattice gas variant) was Michael E. Fisher in 1964. Even though the purpose of Fisher (1964a) was to shoot down classical theories of the liquid-gas critical point, the paper also

between the form of the specific heat and the coefficient of thermal expansion.

<sup>27</sup>Buckingham and Fairbank (1961), p. 81.

<sup>28</sup>Buckingham and Fairbank had an interesting comment:

When it was first discovered, the form of the exact solution for the Ising model came as something of a surprise. Approximate methods of solution yield an apparently second order transition. [...] It is noteworthy that experimental measurements with insufficient resolution also yield an apparent second order transition – and for very similar reasons. A coarse measurement effectively measures what the correspondingly approximate theory can calculate! (Buckingham and Fairbank; 1961, p. 81)

<sup>29</sup>Fisher (1965), p. 95.

<sup>30</sup>The other properties include density distributions in a vertical tube, and the velocity and absorption of ultra sound.

<sup>31</sup>However, “[a] major problem in making accurate measurements near the critical point results from the very high compressibility of the system which causes a partial compression of the medium under its own weight.”(Habgood and Schneider; 1954, p. 98).



compared the numerical results for the lattice gas model with experimental results. The comparison concerned the singularities of the coexistence curve, the specific heat, and the compressibility. He wrote that the shape of the coexistence curve may “be studied theoretically for more-or-less idealized models of a fluid.”<sup>32</sup> Because the Lenz-Ising lattice gas model is “[t]he only model so far sufficiently tractable to yield significant predictions in the critical region [...]”<sup>33</sup>, he chose to compare that model with experimental results.

On the experimental side, he chose the “very careful study of xenon”<sup>34</sup> by Weinberger and Schneider. They confirmed the result by Guggenheim (1945) that the difference between the density of the liquid  $\rho_L$  and gas  $\rho_G$  is given by

$$(\rho_L - \rho_G)/2\rho_c = A(1 - T/T_c)^\beta, \quad (T \rightarrow T_c), \quad (8.2)$$

with  $\rho_c$  the critical density and  $A$  a constant. Fisher analysed their data and found that the exponent equals

$$\beta = 0.345 \pm 0.015. \quad (8.3)$$

This value of  $\beta$  agrees reasonably well with the bounds  $0.303 \leq \beta \leq 0.318$  for this exponent given by the best numerical results for the three-dimensional lattice gas model of the time. Fisher concluded that it is “remarkable, and perhaps unexpected”<sup>35</sup> that the simple lattice gas model gives results so close to these experimental data for the coexistence curve. He continued: “The agreement suggests that in the critical region the lattice gas represents rather adequately the pertinent features of a real gas.”<sup>36</sup> Along with conclusions about the specific heat drawn by Fisher and Yang (discussed below), this was the first statement about the adequacy of the Lenz-Ising model. Fisher immediately pointed out an important lesson: “It appears that only the grosser features of the model - in particular the dimensionality and the short range of the forces - are really essential for obtaining a good description of critical behavior.”<sup>37</sup> So, it is obvious that Fisher found that the Lenz-Ising model was capable of giving insight into real systems. However, he continued, the model is not perfect:

It seems probable, nonetheless, that the difference of about 0.025 between the experimental and theoretical values of  $\beta$  is a real discrepancy due, presumably, to the more artificial aspects of the Ising Hamiltonian which, in particular, restricts the molecules to the lattice positions. There remains the theoretical problem of calculating  $\beta$  for more realistic continuum models. (Fisher; 1964a, pp. 947-8)

Turning to the isothermal compressibility  $\kappa_T$ , it is characterised by an exponent  $\gamma$  defined by

$$\kappa_T = \frac{A}{(T - T_c)^\gamma}, \quad (T \rightarrow T_c^+), \quad (8.4)$$

where  $A$  is constant. Fisher (1964a) compared experimental data by Habgood and Schneider (1954) on xenon with a curve for the lattice gas model obtained by using the numerical value  $5/4$  for  $\gamma$ . He concluded that the theoretical curve “is evidently quite consistent with the experimental points near  $T_c$ .”<sup>38</sup> He did not, however, ascribe much significance to the

<sup>32</sup>Fisher (1964a), p. 947.

<sup>33</sup>Fisher (1964a), p. 947.

<sup>34</sup>Fisher (1964a), p. 946.

<sup>35</sup>Fisher (1964a), pp. 947-8.

<sup>36</sup>Fisher (1964a), p. 947.

<sup>37</sup>Fisher (1964a), p. 947.

<sup>38</sup>Fisher (1964a), p. 949.

fit:<sup>39</sup>

Despite the ‘good fit’ one should not be too impressed! If one looks more closely at the data (especially near  $T_c$ , where the experiments are most difficult and the errors introduced by the numerical differentiation involved in deriving  $\kappa_T$  from the data), one finds they are somewhat irregular. One may, preferably, attempt to calculate a value of  $\gamma$  directly from the data. Although one can conclude with reasonable confidence that  $\gamma_{\text{xenon}} > 1.1$ , the results prove rather indeterminate and one must conclude that more experimental data are needed. One may hope that these will be forthcoming. (Fisher; 1964a, p. 88)

For argon and oxygen such precise measurements became available in the early 1960s due to the work of Voronel’ and his group at the Institute of Physical and Technological Measurements in Moscow. These measurements played an important part in the development.<sup>40</sup> In their paper of 1962 on argon, Bagatskii, Voronel’ and Gusak<sup>41</sup> concluded that the specific heat  $C_V$  of argon behaves like

$$C_V = A^\pm \ln |T - T_c| \quad (8.5)$$

in the neighbourhood of the critical point with  $A^+$  and  $A^-$  for the branches below and above  $T_c$ , respectively. Their conclusion seems to have been generally accepted,<sup>42</sup> except by Fisher, as we shall see shortly.<sup>43</sup>

The results of Voronel’ and co-workers were compared in 1964 with the Lenz-Ising model by Fisher on the one hand and C. N. Yang and his brother C. P. Yang on the other. Fisher devoted an entire paper to the comparison. From an analysis of the experimental results he reached the following conclusion. The specific heat  $C_V$  below  $T_c$  over the two decades from 0.06% to 6% within  $T_c$  is fitted quite well by a logarithmic function. However, above  $T_c$  a better fit is obtained by assuming the following form of  $C_V$ :

$$C_V(T) \approx A/\alpha |1 - (T/T_c)|^{-\alpha} + B_\alpha, \quad (8.6)$$

with a small positive exponent  $\alpha$  (less than 0.1). For the lattice gas model, the specific heat is best described on *both sides* of the critical temperature by a power law with an exponent  $\alpha$  equal to 0.20. That is, the specific heat (for the fcc lattice) is given by,

$$C_V(T) \approx 0.548 |1 - (T/T_c)|^{-1/5} - 0.612 + \dots \quad (T \rightarrow T_c) \quad (8.7)$$

He continued:

Surprisingly, it [the specific heat curve for the three-dimensional Lenz-Ising model] seems to give an excellent representation of the experimental data as close to the critical point as they go, i.e., to within 1 part in 10 000  $T_c$ . (It will be noticed, however, that the measured points do lie some 5 to 10% below the theoretical curve in the range 0.4 to 1.5% above  $T_c$ .) (Fisher; 1964b, p. A1603)

<sup>39</sup>Here I quote from the review Fisher (1965) rather than the initial source Fisher (1964a) because the former is more pedagogical on this point.

<sup>40</sup>In 1964, Fisher wrote that even though it had been known “for some time” that the specific heat at constant volume in the neighbourhood of the critical point shows anomalous behaviour, “[f]urther details of the critical behavior, however, have been revealed only in recent experiments by Voronel’ and co-workers on argon [...] (and, more recently, on oxygen [...]).” (Fisher; 1964b, p. A1599).

<sup>41</sup>Bagatskii et al. (1963). Translated into English the following year.

<sup>42</sup>At least by Yang and Yang (1964) and Chase et al. (1964).

<sup>43</sup>This refers to Fisher (1964b). A few years later, he wrote that  $C_V$  tends to infinity “in a roughly logarithmic manner” (Fisher; 1967, p. 626).

For temperatures below  $T_c$ , the series expansions shows a singularity “probably not much sharper”<sup>44</sup> than logarithmic. So he plotted a logarithmic specific heat curve in the same graph as the experimental curve, and concluded that the slopes of the two curves agree well. However, the magnitude of the specific heat of the model differs from that found in the experiment: “This discrepancy is well beyond the experimental and theoretical uncertainties and represents a real deficiency of the model.”<sup>45</sup>

In contrast to Fisher, Yang and Yang (1964) assumed that the specific heat of argon (and oxygen) is logarithmic on both sides of  $T_c$ . From a comparison with the lattice gas model they concluded that “[i]t is seen that qualitatively the three-dimensional lattice gas with nearest-neighbor interaction gives a fair description of the critical phenomenon.”<sup>46</sup> Moldover and Little (1965) were even more clear about the agreement between Voronel’ and co-workers’ results and the lattice gas model. After noting the sharp contrast between the experiments and phenomenological theories, they concluded: “However, the behavior is precisely that to be expected for the so-called ‘lattice-gas’ model the liquid-gas transition.”<sup>47</sup> Further, “The measurements on argon then indicate that for a *real* gas the specific heat behaves in manner similar to that of a lattice gas.”<sup>48</sup>

However, also discrepancies between the model and experimental results were found. The curve which showed the largest discrepancy was the critical isotherm, that is the pressure as a function of volume at constant temperature  $T_c$ . Widom and Rice (1955) analysed experimental data for xenon, carbon dioxide, and hydrogen and found that they all fulfil the equation

$$p - p_c = -A|V - V_c|^{g-1}(V - V_c) \text{ at } T = T_c \quad (8.8)$$

with  $g \approx 4.2$ . Gaunt, Fisher and Sykes found that for the Lenz-Ising model this exponent has the value  $5.20 \pm 0.15$  in three dimensions,<sup>49</sup> a quite large deviation.<sup>50</sup>

However, such discrepancies could not take away the feeling that emerged that the model was in surprisingly good agreement with experimental results. Considering the mathematical difficulties experienced with modelling phase transitions, this most have given quite some credence to the model.

### 8.2.4 Magnetism

Even though other ‘Ising-like’ materials were found, the most common ferromagnets did not meet the requirements for being of this type. Since the aim was to understand ‘usual’ critical phenomena such as common ferromagnets rather than the more exotic ones, the

<sup>44</sup>Fisher (1964b), p. A1603.

<sup>45</sup>Fisher (1964b), p. A1604. Fisher continued:

One might argue that the reason the lattice gas specific heat below  $T_c$  is too small is also associated with the one-site character of the hard core since this probably leads to an underestimate of the total possible entropy change.

<sup>46</sup>Yang and Yang (1964), p. 304.

<sup>47</sup>Moldover and Little (1965), p. 54.

<sup>48</sup>Moldover and Little (1965), p. 54, emphasis in the original.

<sup>49</sup>Gaunt et al. (1964). Based on a non-rigorous relation between exponents, Widom (1964) had previously derived the result that for the three-dimension lattice gas  $g = 5$ . He was unable to tell whether the discrepancy between  $g = 4.2$  and  $g = 5$  was due to the inadequacy of the lattice gas model or to the relation.

<sup>50</sup>They attributed this discrepancy between the experimental result and the lattice gas model results to the “artificial ‘rigidity’ of a lattice gas with single-site hard cores.” (Gaunt et al.; 1964, p. 715).

finding of these 'Ising-like' materials did not matter much to scientists interested in the relevance of the model to critical phenomena.

The first sign that the Lenz-Ising model might agree with typical magnetic materials, came in 1960 when W. K. Robinson and S. A. Friedberg of Carnegie Institute of Technology in Pittsburgh, reported measurements of the logarithmic specific heat of two hydrated paramagnetic salts ( $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$  and  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ ) which exhibit antiferromagnetism.<sup>51</sup> Their conclusion was that the magnetic contribution to the specific heats for both materials are consistent with a logarithmic singularity at the Néel point, i.e. the transition point of an antiferromagnet. As they remarked, the two-dimensional Lenz-Ising model is known to reveal a logarithmic singularity and it is possible that this is also the case for the three-dimensional model. However, this point does not seem to have been appreciated.<sup>52</sup>

In what appears to be the most thorough comparison of models and experiments in the area of magnetism of the time,<sup>53</sup> Domb and A. R. Miedema (the latter of Kamerlingh Onnes Laboratory in Leiden) looked at three groups of magnets: ferromagnets, cobalt tutton salts, and antiferromagnets. Their goal was to examine whether or not the Heisenberg model and the Lenz-Ising model agree with experimental data. They only confronted a model with data of a material if there were theoretical reasons to expect an agreement between the two.

They did not compare the Lenz-Ising model with materials of the two core areas of critical phenomena within magnetism, namely ferromagnetism and antiferromagnetism. The reason is probably that they found that there are no theoretical reasons for such a comparison. They did note that the model should be able to describe anisotropic antiferromagnets such as  $\text{CoF}_2$  well, but they did not perform a detailed comparison. They did confront the model with so-called cobalt tutton salts,<sup>54</sup> whose magnetic behaviour is anisotropic near 1°K. Susceptibility data show that there is a plane where the crystals of the salts are antiferromagnetic while they are ferromagnetic in the direction perpendicular to this plane. This anisotropy should therefore make the Lenz-Ising model suitable for modelling such physical systems. Indeed, they found a fair agreement.

From their comparison, they concluded:

We may first express moderate satisfaction at the agreement achieved between theory and experiment. Substances have been identified for which either the Ising or the Heisenberg model can be regarded as a reasonable first approximation, and available experimental data on the thermal and magnetic properties of these substances are in fair agreement with theoretical predictions. (Domb and Miedema; 1964, p. 339)

So, they certainly did not conclude that the Lenz-Ising model is in agreement with experiments on ferromagnets. G. B. Benedek was more outspoken. Indeed he concluded, from a comparison between the model and experimental data, that the Lenz-Ising model is not a good representative of ferromagnets:

<sup>51</sup>Robinson and Friedberg (1960). Skalyo and Friedberg (1964) reported measurements with higher temperature resolution on  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ .

<sup>52</sup>In the two theoretical papers published before 1965 which discuss Robinson and Friedberg's results, the first (Domb and Sykes (1962)) did not mention the logarithmic singularity. The second, Fisher (1964a) did mention this, but without comments. This is quite remarkable considering the fact that the papers were written by the pioneers of the application of the Lenz-Ising model.

<sup>53</sup>Even though they had a disclaimer that their experimental data material was not exhaustive, they referred to a remarkable number of results.

<sup>54</sup>They mention five such salts:  $\text{CoK}_2(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{CoK}$ ,  $\text{CoNH}_4$ ,  $\text{CoRb}$  and  $\text{CoCs}$ .

Since 1961-1962 a considerable amount of experimental data on the equilibrium properties of magnetic systems has been obtained. [...] [By] and large the experimental results indicate that the Ising model is inadequate to describe a real ferromagnet. The Heisenberg Hamiltonian has been used successfully to calculate the divergence of the susceptibility and the results are in very good agreement with the experiment. (Benedek; 1966, p. 48)

On the basis of this he continued to discuss the needs in the future:

On the theoretical side, the clear need is a calculation of the magnetization, the critical isotherm, the susceptibility below  $T_c$  and the specific heat using the Heisenberg Hamiltonian. And finally, the close analogy between the fluid and the ferromagnet, combined with the clear breakdown of the conventional expansions of the free energy in a power series around  $T_c$  suggest that the behavior of three-dimensional ferromagnets and fluids near the critical point may be a result of some very general property connected with the ordering and is relatively independent of the details of the Hamiltonian of the system. (Benedek; 1966, p. 48)

Regarding magnets, he definitely preferred the Heisenberg model, but his last remarks must apply to the Lenz-Ising model, so he did not dismiss the latter model completely.

For the three-dimensional Lenz-Ising model, Gaunt, Fisher and Sykes calculated the value of the exponent for the dependence of the magnetisation on the field  $H$  with a series expansion. They found its value to be  $1/(5.20 \pm 0.15)$ , which they compared with the value of  $1/(4.22 \pm 0.05)$  found by Kouvel and Fisher (1964) in an analysis of experimental data for nickel.<sup>55</sup> They were not satisfied with the discrepancy between the two values.<sup>56</sup>

There seems to be consensus about this view of the superiority of the Heisenberg model over the Lenz-Ising model when it comes to experimental agreement.<sup>57</sup> All this meant that experimentally, the Heisenberg model was a much better candidate for a model of ferromagnetism. However, in the field of liquid-gas transition the lattice gas model was considered to be in agreement with some important experimental results, but in conflict with others.

### 8.3 The Change

Why did this disinterest in the Lenz-Ising model change to interest, i.e., why did the Lenz-Ising model become perceived as interesting in the 1960s? First of all, this was *not* caused by a change in perception of the realism of the model. The model was still perceived as less realistic than the Heisenberg model or the continuum gas model, so this cannot explain the change. What was the cause then?

<sup>55</sup>Gaunt et al. (1964).

<sup>56</sup>Gaunt and co-workers attributed this discrepancy to the “extreme anisotropy of the Ising spin interaction [...]” Gaunt et al. (1964), p. 715.

<sup>57</sup>Likewise, Kouvel and Fisher (1964) wrote about recent measurements of the initial susceptibility as a function of temperature performed on iron and iron-vanadium alloys (by Noakes and Arrott) and on the ferromagnetic salts  $\text{CuK}_2\text{Cl}_2 \cdot 2\text{H}_2\text{O}$  and  $\text{Cu}(\text{NH}_4)_2\text{Cl}_2 \cdot 2\text{H}_2\text{O}$  that there is a “close correspondence between these susceptibility results and the recent Heisenberg model calculations” (p. A1626). Kouvel and Fisher, in their analysis of previous experiments, concluded that just above  $T_c$  susceptibility results for nickel is in “excellent agreement” with results on the Heisenberg model, but at higher temperatures there is a deviation.

Let us begin by looking at the recollections of one of the protagonists, C. N. Yang, in his “introductory notes” to the first volume of the journal ‘Phase Transitions and Critical Phenomena’:

There was, however, a time in the 1940’s and 1950’s when Onsager’s solution was regarded as a mathematical curiosity with no real physical relevance. One heard in those days of references to ‘contracting the Ising disease’. This feeling disappeared during the 1960’s when it became clear that the lattice gas description of liquid gas transitions does capture much of the essential features of the singularities. (Yang; 1972, p. 3)

So, according to Yang the discovery of the empirical adequacy of the model was responsible for the change in the perception of the Lenz-Ising model. Moreover, he ascribed the change solely to agreement with experimental results for the liquid-gas transition and not to results concerning magnetism. As we have seen, in several instances surprise was expressed that such a simple model as the Lenz-Ising model was in such a good agreement with experimental results. Yang’s assertion, that the agreement between the lattice gas model and experimental results for the liquid-gas was an important factor in changing the perception of the Lenz-Ising model, seems correct. Even though there was not agreement between all measured physical quantities and those of the model (for instance, the exponent for the critical isotherm was far from satisfactory) the agreement was nevertheless perceived as important. In a situation where the mathematical problems with the oversimplified Lenz-Ising model, not to speak of more realistic models, were recognised to be formidable, it seems natural to assume that such an agreement played an important part in the process towards recognition of the significance of the model.

Was the experimental agreement with liquid-gas transition the only factor? Yang himself has raised some objections to this assertion. In 1995, he gave the following reasons for the abandonment of the previous attitude widespread among physicists that the Ising model and similar problems are unimportant:

The situation dramatically changed around 1960 because of several developments: (1) the experimental discoveries [...] of divergences of specific heats near various phase transition points; (2) theoretical work on the critical exponents led gradually to the concept of universality and to some very useful inequalities among the critical exponents; and (3) the proposal of a scaling law [...]. (Yang; 1995, p. 3)

So, in addition to the discovery of the agreement between the model and experiments, Yang added two other factors. Moreover, from his references with respect to item (1) in the quote, it is clear that he now also found that experimental results within liquid helium (by Fairbank, Buckingham and Kellers) and antiferromagnetism (Robinson and Friedberg) played a role in the change. Yang’s assertions of 1995 seems to be a good starting point for a discussion of other factors.

Starting with experimental evidence from other areas, I do not find that these ought to be included. As I have described in the last section, the agreement between the model and liquid helium data was not considered to be of much importance because liquid helium is a quantum mechanical phenomenon and those using the model were mainly interested in *classical* critical phenomena, at least at first. As to antiferromagnets, the connection between Robinson and Friedberg’s experimental results and the model seems to have been

ignored, as I wrote in the previous section. In more general terms, within antiferromagnetism (and ferromagnetism for that matter), the agreement between model and experiment was perceived by early 1960s physicists as less than good. In the words of Benedek: "[...] by and large the experimental results indicate that the [Lenz-]Ising model is inadequate to describe a real ferromagnet."<sup>58</sup> The agreement between such data and the Heisenberg model was found to be much better.<sup>59</sup>

Turning to the first of Yang's two other developments of importance, what he refers to is probably the following: according to the modern universality hypothesis, which appeared in the early 1970s,<sup>60</sup> the decisive factors of the critical behaviour are the dimension and the range of the interaction,<sup>61</sup> while the type of crystal lattice is of much less significance, i.e., whether it is, say, face-centred cubic or simple cubic. In short, only the overall features matter, not the details. Cyril Domb has argued that the hypothesis grew out of the work of his own group with the Lenz-Ising model already in the early 1960;<sup>62</sup> an example is figure 7.1 showing the spontaneous magnetisation of the model. So Domb's 'universality hypothesis' came at a time where it could have influenced the view of the model. Could this version of the hypothesis have affected the view of the model in the following way: if the details of the models are insignificant for their critical behaviour, why not study a simple model rather than a more complicated one? The two might lead to the same physics.

However, I don't think that Domb's hypothesis played a role for the acceptance of the Lenz-Ising model. Firstly, there is no evidence that something similar to the universality hypothesis is applied to justify the model in the mid 1960s. Domb himself did not express such views in the early 1960s to the mid-1960s. Furthermore, how could examinations of the Lenz-Ising model alone be enough to provide such a justification? The modern universality hypothesis is derived from a range of models. The 'universality hypothesis' of the 1960s was derived from the Lenz-Ising model alone, so it does not say anything about the general behaviour of models and therefore nothing about the irrelevance of the details.

I also disagree with Yang's third point – on the importance of the scaling hypothesis of Benjamin Widom. Widom assumed that the equation of state in the neighbourhood of the critical point is a homogeneous function of the density and the temperature. From this hypothesis he derived a linear relation between critical exponents for compressibility, the coexistence curve and the specific heat at constant volume: if the values of two exponents are known, the third can be determined. As we shall see in Chapter 10, Widom did use the Lenz-Ising model to test the hypothesis. However, the model gave credence to the hypothesis rather than the other way round. Therefore, it is hard to see that the scaling hypothesis played an important part in the considerable change in the attitude towards the relevance of the model.

Stephen G. Brush has put forward yet another proposal for the decisive factor behind the change:

As mentioned above, the Lenz-Ising model was not taken seriously for several decades because it grossly oversimplified the nature of interatomic forces

<sup>58</sup>Benedek (1966), p. 48.

<sup>59</sup>Domb and Miedema (1964).

<sup>60</sup>See Domb (1996).

<sup>61</sup>Whether it is nearest-neighbour or next-nearest does not change anything.

<sup>62</sup>Domb (1996).

and did not seem to correspond closely to any real system, with the possible exception of alloys and binary mixtures. The situation changed dramatically in 1961, [...] when George A. Baker, Jr., at the Los Angeles Scientific Laboratory, [...] showed that a mathematical technique invented by the French mathematician Henri Padé in 1891 could be used to determine the singularities at the critical point from known terms in the series expansions for the Lenz-Ising model. [...] (Brush; 1983, p. 253)

As I understand him, Brush advocated the view that it was the novel application of a mathematical technique, Padé approximants, which changed the situation. The argument seems to amount to something like this: this technique allowed for the determination of previously inaccessible critical behaviour of the model, which could then be compared with experiments. So, it was the lack of reliable results for the model which impeded a confrontation of the model with experiments. I agree that Baker's method did greatly enhance the number of results, but I disagree that it had a marked effect on the acceptance of the model. Reliable data were available prior to Baker's method, but they were not compared with experiments.

In addition to Yang's and Brush's points, we should also examine whether the focus on the similarities between different transition points played a role. In his monograph of 1956, Temperley remarked that "[...] the basic resemblances between apparently unrelated types of transition have only come to light gradually during the course of many years."<sup>63</sup> Indeed, one of his main reasons for writing the book was "to call attention to some of these resemblances and, at the same time, to try to pin-point the individual peculiarities of each type of transition."<sup>64</sup> That the Lenz-Ising model could represent several such different systems were recognised already in the 1930s and when the experimental similarities between such systems were at last recognised, the theoretical status of the model was strengthened. However, even though the realization of the similarities of different systems seems to have emerged in the last half of the 1950s, the Lenz-Ising model did not receive much attention. This shows that this development did not play as important a role in the acceptance of the model as did the agreement with experiments. This point is illustrated by the fact that Temperley in his book did not describe the Lenz-Ising model as a general model of phase transitions.

To sum up, I believe that what was decisive for the change of the perception of the Lenz-Ising model was the agreement of the model with experiments which had emerged in the late 1950s and early 1960s. The main factor behind the change seems to be the experience that there was good agreement between the model and experiments. Moreover, it was the experimental results within classical gases which were crucial. However, this changed the situation for the model as a representative of magnets as well.

<sup>63</sup>Temperley (1956), p. vii. However, a few years before, Tisza (1951) wrote about second order phase transitions: "That these transitions reveal common thermodynamic features has been frequently recognized, although the underlying molecular mechanisms were of an unusual diversity."(Tisza; 1951, p. 2).

<sup>64</sup>Temperley (1956), p. vii.





# 9

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## The Mayer Model of Gases

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The last chapter showed that in the early 1960s a change occurred in the perception of the Lenz-Ising model: the model was ‘suddenly’ perceived as physically relevant. It was also mentioned that the Heisenberg model was the preferred model in the field of magnetism in the 1950s. The present chapter documents that the so-called Mayer model was the preferred one in treating condensation of gases in the 1950s. However, in the second half of the 1960s, the Lenz-Ising model had, by and large, taken the place of the Mayer model, while the Heisenberg model was still perceived as interesting and on par with the Lenz-Ising one. Since the Heisenberg model was not toppled by the Lenz-Ising model – rather the two models coexisted – it is interesting to look at why, by and large, the Mayer model was abandoned in the 1960s. The development of the Mayer model is the topic of the present chapter, which gives an answer to the question: why did the Lenz-Ising model topple the Mayer model? Was it due to defects of the latter model or was it because of the merits of the Lenz-Ising model?

This chapter attempts to do three things: first, document that the Mayer model was perceived as the physically relevant model of gas condensation in the 1950s; second, discuss why the model fell out of focus in the following decade; and thirdly, provide a basis for a discussion of different approaches to modelling (in Chapter 12). This is not at all meant as an exhaustive discussion of the Mayer model but as intended to provide enough material for pursuing these three points.

The historical development of Mayer’s model and method has been described briefly by previous authors, with an emphasis on the very general aspects of the model and on its reception.<sup>1</sup> Here a more thorough examination of the development in the perception of the model will be made.

### 9.1 The Mayer Model

The American scientist Joseph E. Mayer (1904-1983) did research on condensation and critical points from 1937 to the 1960s, but discontinuously. Here we shall look at his theory from the late 1930s, its at first positive and then negative reception, and then a simplification of his original model, made in collaboration with Teresa Ree Choy<sup>2</sup> and her brother Francis Ree, published in three papers of the 1960s.

In general, Mayer’s research was in the borderland between chemistry and physics. He was trained as a chemist and received his Ph.D. degree from UC Berkeley in 1927 under the supervision of Gilbert N. Lewis. The research reported in the dissertation was – as

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<sup>1</sup>See Brush (1983), pp. 246–250, Hodderson, Shubert, Heims and Baym (1992), pp. 523–524, and Domb (1996), pp. 195–197.

<sup>2</sup>Who later changed her last name to Chay.

was usual in chemistry at that time – experimental.<sup>3</sup> In fact, Mayer, whom many see as a *theoretical* chemist, considered himself “an experimentalist even into the 1950’s, although I guess that most of those who recognize my name at all think of me as a ‘sadistical mechaniker.’”<sup>4</sup> However, it is his theoretical work that interests us here. In addition to the statistical mechanics of gases, Mayer’s theoretical work also dealt with the application of statistical mechanics to solutions and with thermodynamics of ionic crystals. In view of his mastery of statistical mechanics – his book on the subject with his wife Maria Goeppert Mayer (first edition in 1940) is widely acclaimed – it is remarkable that Mayer taught himself this discipline as a postdoctoral fellow with Lewis in 1928-1929. There were no graduate courses in chemistry, but the students were encouraged to take classes in physics and mathematics.<sup>5</sup> Mayer has recalled that the training at Berkeley focused on general aspects:

I think that the emphasis, which we soon began to recognize, on problems of general importance rather than on adding only one more example to many similar worked out and well understood cases, was probably the prime characteristic that we, as students, took away from our experience at Berkeley as our most important legacy. (Mayer; 1982, p. 10)

Mayer spent his professional life at various chemistry departments throughout the US: John Hopkins (1930-39), Columbia (1939-45), Chicago (1946-60), UC San Diego (1960-72) and then as a professor emeritus at UCSD until his death.

### 9.1.1 Mayer’s First Treatment of Condensation

In 1937, Mayer published a paper on imperfect gases and their condensation. This paper led to an avenue of research, not only by Mayer and collaborators but also by other groups, mainly Boris Kahn and George E. Uhlenbeck, on the one hand, and Max Born and Klaus Fuchs (the latter is mostly famous for his conviction in 1950 of being a spy for the Soviet Union) on the other. This research was directed at a theoretical understanding of the statistical mechanics of gases condensing to the liquid state. Thus the focus was not on the specific phase transition occurring at the critical point. Since the critical point is the main subject of this dissertation it is natural to ask why, then, this research on condensation is discussed. There are several reasons. First, as we shall see, the critical point does actually play a significant role in the work and one of Mayer’s papers (with his co-author Sally Harrison<sup>6</sup>) is devoted to this transition. Second, Mayer’s model and method and its extensions were the subject of a great discussion in relation to approaches more specifically concerned with critical points. Oscar K. Rice, for instance, examined some of Mayer’s predictions about the critical point thoroughly for a period of many years. Third, the Yang and Lee theory published in 1952 is widely discussed and I shall argue that this theory can be seen as a successor to Mayer’s treatment. Fourth, Mayer’s treatment and the Yang and Lee theory appear to be the only statistical mechanical theories of condensation in the period just before the 1960s that received some attention. In order to illustrate the considerable change in the approach to critical phenomena in the 1960s, it is interesting to compare with these theories, only a few years older. This is the subject of Chapter 12.

<sup>3</sup>Mayer (1982).

<sup>4</sup>In letter to B. S. Rabinovitch, MSS 47, Box 2, Folder 8.

<sup>5</sup>Mayer (1982).

<sup>6</sup>Harrison and Mayer (1938).

The following is a short presentation of the main ideas in the treatment with the focus on the physical assumptions rather than on the mathematical aspects of the treatment.

Already Born and Fuchs, in 1938, pointed out that Mayer's work broke new ground because it treated phase changes from an entirely new point of view, starting from the gas phase rather than from an assumption of the coexistence of phases characteristic of the older theories.<sup>7</sup> In contrast to these other theories, Mayer's treatment allowed to pose the question, in Born and Fuchs's formulation, 'How do the gas molecules know when they have to condense?' and Mayer's treatment was the first attempt to obtain an answer. Even though Mayer's work was new it did build on ideas by the British mathematician Ursell in the 1920s,<sup>8</sup> and the French Jacques Yvon had similar ideas at roughly the same time, but his work was less well known.<sup>9</sup>

The most explicit description of the overall purpose of the treatment of Mayer and successors was not given by Mayer himself but by Kahn in his dissertation of 1938:

First of all, one requires a theory that can explain the general qualitative features of behaviour of gases and liquids. The most striking of these features is the existence of sharp phase transitions (condensation and evaporation). This means mathematically that the equation of state cannot be represented by one analytical function but consists of *several analytically different parts*. Since this property is common to all substances one would expect it to be possible to give a very general explanation demanding no exact knowledge of the interactions between molecules, since this is different for every substance. (Kahn; 1938, p. 1, emphasis in the original)

Mayer subscribed to this programme and took some steps towards its fulfilment (which has not been achieved yet). He and his co-workers derived an equation of state for a system composed of  $N$  identical molecules. This treatment should be based on statistical mechanics and the aim was to do "without arbitrary physical or mathematical assumptions."<sup>10</sup> However, they wrote, the system had to be limited to have specific properties if such a treatment were to be feasible. Consequently, they introduced three fundamental assumptions or limitations, which are "absolutely essential."<sup>11</sup> They are:

[...] first, that the masses of the particles making up the system are large enough so that the classical laws of mechanics are applicable at the temperatures and volumes we wish to investigate; second, that the mutual potential between particle pairs falls off with the fourth or higher power of the distance between the pairs; and third, that the total potential energy of the system is representable as the sum of the potentials between pairs of particles which depend only on the differences of the coordinates of the pairs. (Mayer and Harrison; 1938, p. 87)

Only the last assumption was further justified. They observed that this assumption is "equivalent to restricting the system to one composed of chemically saturated molecules incapable of forming true valence bonds with each other."<sup>12</sup> This assumption does not

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<sup>7</sup>Münster (1969), p. 559.

<sup>8</sup>See Brush (1983).

<sup>9</sup>Domb (1996), p. 196.

<sup>10</sup>Mayer and Harrison (1938), p. 87.

<sup>11</sup>Mayer and Harrison (1938), p. 87.

<sup>12</sup>Mayer and Harrison (1938), p. 87.

imply that collisions between more than two molecules are neglected; such collisions are allowed, but they are split into a sum of interactions between pairs of molecules. Mayer and co-authors did not argue for the common assumption of the interaction between pairs, but in 1958, he gave the following description of this assumption:

Although the simple derivations of the quantum mechanical origin of this potential always give the pair interactions the leading terms, there is no compelling reason for assuming that the specific three-body interactions can actually be neglected, especially in view of the greatly increased number of these over the pair interactions in a condensed system. (Mayer; 1958, p. 22)

So, the assumption may not be as innocent as it looks at first, but it is common to make it nevertheless.

Returning to the papers of the 1930s, they involved some inessential limitations as well. However, since these assumptions are not fundamental and can be removed at the cost of a more complicated examinations, they will not be considered here.<sup>13</sup> As we saw in Fisher's description of the assumption in chapter 8, the assumptions above were not perceived to be too unrealistic.

Mayer and co-authors avoided giving a name for their treatment and simply referred to it as the statistical mechanics of condensing systems. Some of their successors called it 'Mayer's theory.' Considering its general nature and scope this appellation is natural. However, it plays down the fact that the theory contains non-trivial *ad hoc* assumptions and so could equally well, if not better, be called a model. I shall use the name 'the Mayer model' for these assumptions about the  $N$  particle system in order to underline this perspective, while I shall call the theory based on this model 'Mayer's treatment'<sup>14</sup> and thus avoid using the term 'Mayer's theory' in the following. Finally, the way Mayer examined the model mathematically shall be called 'Mayer's method.'

From statistical mechanics and the assumptions introduced above, Mayer and co-workers were able to rigorously derive a series governing the behaviour of the model. From equally rigorous considerations of the convergence radius of this series, they were able to show that two volume values exist,  $v_f$  and  $v_s$ . Between these two values both the Gibbs free energy  $F$  and the pressure  $P$  are independent of volume. This means that there is a range of feasible volumes for the same value of  $F$  and  $P$ , i.e. the coexistence of phases. From this they concluded: "This constancy of  $P$  and  $F$  for  $v_f \leq v \leq v_s$  may be considered to be the thermodynamic criterion of a change of phase."<sup>15</sup> Moreover, they identified  $v_f$  with the volume per molecule of the condensed phase and  $v_s$  with the volume per molecule of the vapour. The situation is illustrated in the shaded area of figure 9.1. In this area the fluid (liquid) phase and the vapour phase will coexist. In short, Mayer and Harrison were able to show in a rigorous manner that the model exhibits a phase transition.

In addition, they also made some predictions based on a non-rigorous arguments. First, they showed that above a certain temperature  $T_c$  the argument leading to the existence of  $v_f$  breaks down. This means that the proof of the occurrence of condensation

<sup>13</sup>Mayer and Harrison (1938), p. 87. These limitations are the following: a) The molecules are identical; b) the number of molecules  $N$  is so large that terms of the order  $N^{-1/3}$  can be ignored compared to unity; and c) the only degrees of freedom of the molecules are the translational ones.

<sup>14</sup>It should be noted that, for the sake of brevity only, I have omitted the names of Mayer's co-authors, Philip Ackerman and Sally Harrison from this appellation.

<sup>15</sup>Mayer and Harrison (1938), p. 92.

also breaks down. Since the characteristic feature of critical points in real liquid-gas systems is that no condensation occurs at temperatures above it, they point out that “[o]ne is immediately tempted to identify  $T_c$  with the critical temperature.”<sup>16</sup> However, it should be stressed that they did not rigorously prove that above this temperature there is no condensation in the model; they only showed that the *argumentation* for the existence of condensation breaks down. At any rate, they identified  $T_c$  with the critical temperature.

Next, they argued for the existence of a hitherto unknown temperature,  $T_m$  below the critical point where the equations predict some unexpected phenomena. The definition of the critical point, as given above, is usually found to coincide with the disappearance of the surface tension of the liquid, so that below the critical temperature the two phases are visibly distinguishable. However, Mayer and Harrison found that the latter temperature differed from the critical temperature  $T_c$ . They denoted the new temperature  $T_m$ . For temperatures between  $T_m$  and  $T_c$  there will be two phases, but there is no visible sharp meniscus separating the two phases. For temperatures below  $T_m$  the usual or expected behaviour is resumed. The shaded area for temperatures between  $T_m$  and  $T_c$  is called the “Derby hat region.” Prior to the work of Mayer and Harrison,  $T_m$  had been regarded as identical to  $T_c$  “by most theoretical workers.”<sup>17</sup> Thus, the model was the main vehicle for the discovery of this temperature, but the argument was not rigorous.

Their following article,<sup>18</sup> was devoted exclusively to a discussion of the experimental basis of this hitherto unnoticed temperature. With the starting point in the sketch reproduced in figure 9.1, they recapitulated their attitude towards the justification of their results:

The part of the diagram to the right of  $V_c$ , and all of it above  $T_c$ , is deduced strictly from the equations of the previous article [i.e., Mayer and Harrison (1938)]. The portion to the left of  $V_c$  and below  $T_c$  represents a logical guess from the nature of the kinetic picture deduced from these equations. The authors, however, are less certain of the details of this portion of the diagram. (Mayer and Harrison; 1938, p. 101)

Harrison and Mayer were able to convince several others that there is good experimental evidence for a distinct  $T_m$ , but this was the subject of a lot of discussion and when the issue was eventually settled, in the early 1950s, the existence of  $T_m$  was actually dismissed.<sup>19</sup>

In general, Mayer and his co-authors confronted their theoretical results with experimental evidence. For example, Mayer and Ackerman compared numerical predictions for the quantities such as  $PV/RT$  and  $P$  with experimental values for  $\text{CO}_2$  and  $\text{CH}_4$ . They obtained moderate agreement, for which they concluded “The agreement between the calculations and the experimental values is not unencouraging.”<sup>20</sup>

To sum up, Mayer and collaborators provided a reasonable model for which they could show in rigorous manner that it exhibits a phase transition. In addition to this result, they provided several others, but on a non-rigorous basis. The most important was the prediction existence of a hitherto unknown temperature  $T_m$ , because it led to much further research.<sup>21</sup>

<sup>16</sup>Mayer and Harrison (1938), p. 93.

<sup>17</sup>Mayer and Harrison (1938), p. 95.

<sup>18</sup>Harrison and Mayer (1938).

<sup>19</sup>See Brush (1983).

<sup>20</sup>Mayer and Ackermann (1937), p. 74.

<sup>21</sup>Brush (1983).

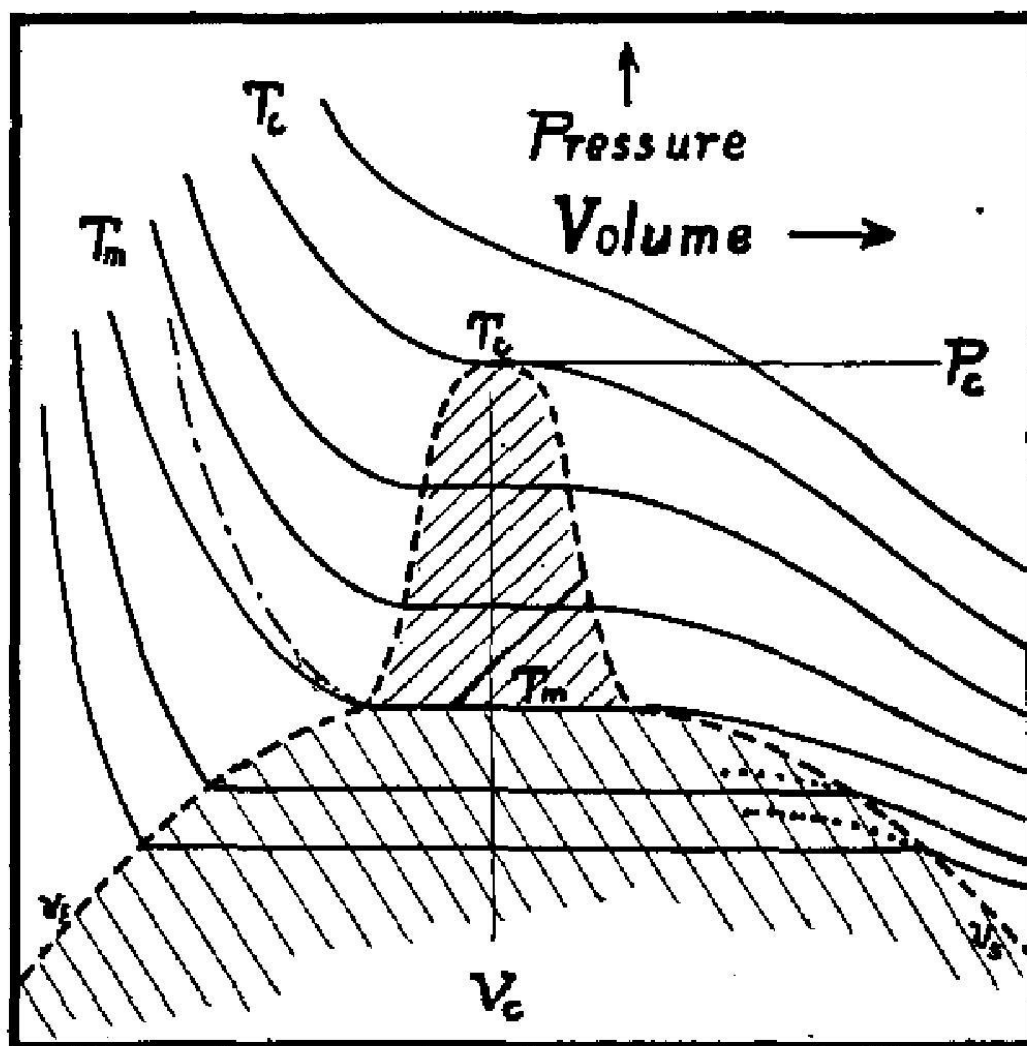


Figure 9.1: Figure from Harrison and Mayer (1938).

### 9.1.2 Yang and Lee's Theory

Despite its apparent success in demonstrating the exhibition of condensation in the model, Mayer's treatment was soon found to be unable to lead to further progress. It was pointed out in 1952 that Mayer's treatment cannot deal with the liquid phase, and afterwards it was generally recognised that the method can only show the existence of a condensation point, but not predict the behaviour in the beyond the condensation point. The problem is that no analytic continuation of the series governing the thermodynamic behaviour is possible beyond the singularity on the positive real axis. This deficiency is due to the application of the so-called cluster expansion to the model, rather than to the model itself and so says nothing about the latter.<sup>22</sup> "Thus, even in the most favorable cases the Mayer theory [i. e. Mayer's treatment] can only yield an incomplete picture of condensation,"<sup>23</sup> and Mayer's treatment does not determine the position of the condensation point and the nature of the singularity.<sup>24</sup> However, it should be stressed that nobody questioned the validity of the model; it was Mayer's method which was found to be insufficient. The problem with the method is that it is not capable of yielding the equation of state for the liquid phase. Two papers of 1952 by C. N. Yang T. D. Lee are exemplary for a discussion of the perception of Mayer's model and his method.<sup>25</sup> They provided a new treatment (of a model almost identical to Mayer's) which remedied some of the shortcomings of Mayer's method, and they introduced the lattice gas model and discussed it thoroughly. I shall mainly be concerned with their criticism of Mayer's work.

In the introduction, Lee and Yang wrote that the latter's work on the spontaneous magnetisation of the two-dimensional Lenz-Ising model led them to consider the lattice gas model. From this model they went on to examine the deficiency of Mayer's method. The problem is Mayer's method rather than his model because "this difference lay, not in the difference of the models, but in the inadequacy of Mayer's method for dealing with a condensed phase."<sup>26</sup> In fact, even though they thought that the behaviour of the lattice gas model "in many ways should reveal the features of an actual gas"<sup>27</sup>, their method applied to a model very similar to Mayer's. Instead of Mayer's fourth power decay of the interaction, they assumed that the interaction  $u$  as function of distance  $r$  has a finite range  $b$  so that

$$u(r) = 0 \text{ for } r \geq b \quad (9.1)$$

and  $u(r)$  is nowhere minus infinity.

The main gist of their first paper was to provide a necessary condition for the occurrence of phase transitions in systems satisfying these assumptions. Based on the obtained necessary condition, they were able to characterise the breakdown of Mayer's method. They concluded that this method is mathematically incorrect in the whole liquid region due to an unjustified replacement of a volume dependent quantity with its value in the limit of infinite volume. This defect could be remedied, but most of the treatment would have to be discarded.

In his textbook a few years later, T. S. Hill weighed advantages and disadvantages of Mayer's treatment against the one by Yang and Lee:

<sup>22</sup>See Münster (1969), p. 568.

<sup>23</sup>Münster (1969), p. 568.

<sup>24</sup>Münster (1969), p. 568.

<sup>25</sup>Lee and Yang (1952) and Lee and Yang (1952).

<sup>26</sup>Yang and Lee (1952), p. 404.

<sup>27</sup>Yang and Lee (1952), p. 404.



The formalism of Ursell and Mayer [...] is developed in a straightforward way, with the intermolecular force between pairs of molecules occupying an obvious and important role from the outset. However, this approach has the disadvantage that the theory must be carried through mathematically complicated and sophisticated stages before condensation and the liquid state can be included in a rigorous way. In fact, this part of Mayer's theory has not yet been completed. On the other hand, Yang and Lee have suggested an alternative formalism in terms of which a rigorous mathematical discussion of condensation and the liquid state can be included as easily as a discussion of the gas phase. But the connection with intermolecular forces becomes very remote in this theory. In fact, the theory is sufficiently general that the form of the configuration integral is never made use of. (Hill; 1956, pp. 169-170)

So, Mayer and Yang and Lee, by and large, agreed about the fundamental assumptions, but they provided different methods to cope with the models. Whereas Mayer's method seemed stuck in problems, Yang and Lee's new method provided new fuel for the hope of succeeding in basing a theory of condensation on these fundamental assumptions rather than the crude lattice gas model. For instance, Louis Witten published a paper two years later on a generalisation of their treatment.<sup>28</sup>

### 9.1.3 Mayer's Simplification in the 1960s

In the 1960s, Mayer returned to statistical mechanics of critical points and resumed his work on condensation and critical points of one-component systems with co-workers Choy and Ree. The fundamental model was the same, but he and collaborators, who did much of the work, used new techniques and new approximations.

While this treatment far from received the attention of the treatment of the 1930s, it is significant because it shows that Mayer did not change to the lattice gas model in the 1960s, but kept focussed on something very similarly to his original model.

The results of Mayer and collaborator's research project were published in three papers.<sup>29</sup> The starting point of all three was the same fundamental system as that of Lee and Yang. Thus, except for the replacement of the assumption of the model of the 1930s – that the interaction falls off with the fourth or higher power of the distance – with the assumption that the interaction is short-ranged, the model of the 1960s was identical to the one of the 1930s. However, after having derived some general relations of this system, they restricted their treatment to a "simple model".<sup>30</sup> I shall not discuss these restrictions in any detail, but only note that even though they are non-trivial, they are not too unrealistic.

One of the purposes of the first paper was an attempt to explain the fact, found by Voronel' in argon,<sup>31</sup> that the specific heat diverges at the critical point.<sup>32</sup> What do Choy and Mayer mean by explanation? The only thing which can count as such in their paper is the establishment of a relation between the divergences of the thermodynamic functions and functions describing the configurational probabilities. However, they were not able

<sup>28</sup>Witten (1954).

<sup>29</sup>Choy and Mayer (1967), Choy (1967) and Choy and Ree (1968).

<sup>30</sup>Choy and Mayer (1967), p. 110.

<sup>31</sup>Bagatskii et al. (1963).

<sup>32</sup>Choy and Mayer (1967), p. 111.

to obtain a numerical value for the exponent of the specific heat anomaly. The goal to explain the specific heat anomaly they shared with people subscribing to the lattice gas model, but they chose quite another model to achieve this goal.

Another example of a shared goal is the so-called critical exponent relations. In the 1960s, several relations between the critical exponents characterising different critical behaviour of a particular system were put forward,<sup>33</sup> for instance between the exponent of the specific heat of a gas, its compressibility and its coexistence curve. These relations did not follow rigorously from theory, so they were only conjectured and constituted a major topic for physicists interested in critical phenomena in general. Mayer and Choy shared the interest in such relations with scientists working on critical phenomena in general. In fact, Choy obtained a relation previously found by Leo P. Kadanoff in a famous paper:<sup>34</sup> “This conclusion is identical to a formula proposed by Kadanoff with the scaling laws for Ising models.”<sup>35</sup> It is strange that her derivation did not lead to more interest, since it was a completely different way of obtaining the scaling laws to those of Kadanoff’s.

The work described above illustrates that some researchers, *in casu* Mayer, did not give up the attempt to explain critical points in terms of a more realistic model than the lattice gas model and even in the late 1960s he seriously considered the continuum gas model. Thus, the lattice gas approach was not the only approach available at this time. Furthermore Mayer and his collaborators shared with their contemporaries the interest in critical exponent relations and in explaining critical point singularities, but they considered very different models to the lattice gas model.

#### 9.1.4 The Views of the Mayer Model from the 1930s to the 1960s

##### The reception of Mayer’s first treatment

There is a lot of evidence that Mayer’s first treatment was received very positively and with great enthusiasm in the 1930s. Boris Kahn and George Uhlenbeck found the treatment promising and Max Born, shortly after the publication of Mayer’s first papers, called his work “a most important contribution to the development of van der Waals theory [...]”<sup>36</sup> Moreover, Domb recalled in 1996:

My first mentor at Oxford, M. H. L. Pryee, has told me that he was present at the colloquium in Cambridge when Mayer’s results were first presented. Fowler, the outstanding world authority on statistical mechanics, was deeply impressed by Mayer’s work, and said that he would not have believed that such progress could have been achieved in his lifetime. The way seemed open for a detailed explanation in atomic terms of the liquid and gaseous phases, the critical point, and the striking discontinuities which occur in the equation of state. (Domb; 1996, p. 196)

However, Pryee’s optimism was not fulfilled (and has not yet been so), and already Born had misgivings about Mayer’s treatment. He found Mayer’s method “rather difficult to understand and his results not completely satisfactory.” Mayer had used an invalid formula

<sup>33</sup>See, e.g., Domb (1996).

<sup>34</sup>Kadanoff (1966).

<sup>35</sup>Choy (1967), p. 4314.

<sup>36</sup>Hoddeson, Shubert, Heims and Baym (1992), p. 524.

for high densities.<sup>37</sup> However, this criticism did not concern Mayer's *model*, that is the fundamental assumptions on which his treatment was based.

### The status of the model in the 1950s

Despite the fact that it was evident that the treatment was flawed, most people seem to share the perception that this treatment was the way, nevertheless, to approach the condensation problem, at least until the early 1950s. This impression is given, for instance, by J. de Boer's paper entitled "Théorie de la condensation" in the section on "Principes Généraux et Condensation" at the conference on phase transitions in Paris in 1952. The paper is an introduction to the subject of condensation, so the approaches it deals with must somehow reflect what de Boer consider to be the significant theories. De Boer discussed almost exclusively Mayer's model, so it is natural to assume that de Boer considered this model to be the most important at the time. However, his remarks about the work by Yang and Lee (not yet published at that time) reveals his reservations concerning that state-of-the-art:<sup>38</sup>

The last paragraph on the theory of condensation shows that at present the theory is still very incomplete and that there is still divergences in opinion among the theorists. Even if we think that we have a 'physical picture' of the condensation process, fundamental research on the problem of condensation is still necessary. (de Boer; 1952, p. 17)

In the 1950s, the model or something very similar was the main approach to condensation. As I observed above, the fundamental assumptions of Yang and Lee's treatment were only marginally different from those of Mayer's. Besides, Benjamin Widom published a paper in 1957,<sup>39</sup> where he examined a model similar to Mayer's (though he added further approximations).

Another example is Temperley's influential book of 1956 on phase transitions. Here he reviewed "five possible liquid models,"<sup>40</sup> which did *not* include the lattice gas model. He concluded that the "most promising lines of approach at present"<sup>41</sup> seem to be "Mayer-type theory"<sup>42</sup> and the so-called distribution function approaches, which need not interest us here. The reason that these two were thought to be the most promising was that the others seem to require some *ad hoc* assumptions. Temperley did discuss the lattice gas model, but as one of two "idealised models for which Mayer's attempted description of the critical region is incorrect,"<sup>43</sup> rather than a model with a say on real liquids.

<sup>37</sup>Hoddeson, Shubert, Heims and Baym (1992), p. 524. Moreover, in order to predict the equilibrium properties from Mayer's equation of state, an *ad hoc* device called the Maxwell construction had to be applied.

<sup>38</sup>In my translation. The original reads:

Ce dernier paragraphe sur la théorie de la condensation montre qu'à présent la théorie est encore très incomplète et qu'il subsiste encore des divergences d'opinion entre les théoriciens. Bien que nous croyions avoir une "peinture physique" du processus de la condensation, des recherches fondamentales sur la problème de la condensation sont encore nécessaires.

<sup>39</sup>Widom (1957).

<sup>40</sup>Temperley (1956), p. 52.

<sup>41</sup>Temperley (1956), p. 52.

<sup>42</sup>Temperley (1956), p. 52.

<sup>43</sup>Temperley (1956), p. 87.

The important thing here is not the exact assumptions of the models, which did in fact differ between these different treatments. Rather, what is interesting is the fact that they did not differ *very much*, so the lattice gas model, in which the gas molecules are restricted to lattice sites, was in quite another category. Compared to the lattice gas model, the assumptions of Mayer's model, and the other models discussed here, were perceived by most physicists as much more realistic. However, attempts to pursue the lead of the Mayer treatment seem to have died out at the beginning of the 1960s. Most people would probably subscribe to the Münster's of 1969: "Because of the unsolved problems and the inherent weaknesses of the Mayer theory [i.e. the Mayer treatment], the numerous attempts to study the problem of condensation for simple models are of interest."<sup>44</sup>

## 9.2 The Preference for the Lattice Gas Model

So, even though the lattice gas model was seriously put on the map in the 1950s by Lee and Yang's paper, this decade seems to belong to models like Mayer's in the area of fluids. Although interest in Mayer's model continued well into the 1960s,<sup>45</sup> the lattice gas model came much into focus as a consequence of the experimental results of Voronel' and collaborators. This was further fuelled by the fact that it seemed practically impossible to obtain numerical results of the Mayer model for, say, the specific heat due to the great mathematical intricacies in the model. This meant that the model moved away from the focus of attention. The model was neither discussed at the NBS conference in 1965<sup>46</sup> nor in the first four volume of the seminal series on "Phase Transitions and Critical Phenomena", edited by Domb and Green in the early 1970s.<sup>47</sup> These four volumes were meant to cover the essentials of the theory. Moreover, Stanley's popular textbook on the same subject did not refer to Mayer's work. However, it should be noted that, as we have seen, Mayer and collaborators kept their focus on the model, but they were a minority.

The waning interest in the model was not due to a realization that the physical principles of the model were wrong. In the words of Münster: "[...] the physical concept [...] underlying the Mayer condensation theory is completely plausible [...]"<sup>48</sup>. The problem lies in the mathematical difficulties involved in manipulating the model, not in its physics. Furthermore, the fact that the lattice gas model was actually in agreement with some experimental facts about the liquids, might have influenced the interest in this model at the expense of the Mayer model. Indeed, in an influential review of 1967 on condensation, J. S. Langer<sup>49</sup> approached this phenomenon through the lattice gas model. The lattice gas model was preferred to the Mayer model. However, the former model had to compete with other models for the appellation 'the preferred model' of condensation. In fact, the Kac model<sup>50</sup> and the droplet model,<sup>51</sup> both received much attention. It would lead to far

<sup>44</sup>Münster (1969), p. 568.

<sup>45</sup>See Münster (1969), pp. 564–566.

<sup>46</sup>Mayer did not participate in the conference, but he had been invited to chair a session. He accepted, but was unable to attend because he had to get a new glass eye. Letter from Mayer to M. S. Green, February 17, 1965. In Joseph Mayer Papers, Mandeville Special Collection, UC San Diego, Box 7, Folder 35.

<sup>47</sup>For the sake of completeness, it should be noted that Yang made a passing historical remark to the model in the first volume.

<sup>48</sup>Münster (1969), p. 564.

<sup>49</sup>Langer (1967).

<sup>50</sup>See Hemmer and Lebowitz (1976) for a review.

<sup>51</sup>See Fisher (1967) for a discussion of this model.

astray to discuss these two models in detail in the present dissertation. Here it suffices to say that they were not found capable of accommodating the overall aspects of condensation. The role of the Kac model was mainly to provide a microscopic model leading to the van der Waals equation known to be quantitatively wrong, while the droplet model was not derived rigorously from a microscopic model. These shortcomings meant that the lattice gas model held a more prominent position than the other two models during the 1960s.

So, in sum, the Mayer model fell out of focus mainly because it was not mathematically tractable. If it had been technically possible to deal with, it is not certain that the lattice gas model would have gained the position it got during the 1960s.

# 10

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## The Role of the Lenz-Ising Model 1960-1965

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Returning to the Lenz-Ising model, as argued in Chapter 8 the realisation of its empirical adequacy changed the perception of the model. How did this affect the role played by the model?

The model was used extensively throughout the 1960s. As before, the overall aim was to explain and understand macroscopic phenomena from microscopic models. However, it was clear in the 1960s that a general systematic account of critical phenomena based on microscopic models alone was not impending. Therefore ideas and *ad hoc* theories<sup>1</sup> about the behaviour of such phenomena, which had not been justified by microscopic models, came into play. Such non-rigorous approaches included the scaling hypothesis and a theory about the scattering of light at the critical point.

This and the following chapter try to span the different roles which the Lenz-Ising model played in the pursuit for insight into critical phenomena. One aspect is left out, however, because it has already been dealt with in chapter 8: the confrontation of the model with experiments. I will not go through them once again, but only refer the reader to that chapter. My main point will be that one should distinguish between the roles played in the two halves of the 1960s. In the first half the model was used in a scattered way for particular purposes, whereas in the second half it was intended to provide a more systematic account of critical phenomena for which it played an indispensable role.

This chapter deals with the variety of different roles played by the model in the first part of the 1960s. All these roles were aimed at specific small-scale tasks.

### 10.1 Model Results as ‘Experimental Results’

Already the year after Onsager’s paper, Wannier concluded that all the approximative methods failed at the critical point because they give a discontinuous specific heat and not an infinite one as in Onsager’s solution of the two-dimensional Lenz-Ising model. This was the first example of the *discarding* ability of the Lenz-Ising model. In the 1960s this ability was put to a good use because conclusive experimental results were often wanting. In such situations the Lenz-Ising model might step in and provide results which could function like experimental data. The model played this role in several papers, among them four papers from 1962 to 1965 by Benjamin Widom. These four papers, dealing with the critical point of liquid-gas, are exemplary for this use of the model. Moreover, they illustrate that in the 1960s the model received attention from circles outside the King’s College group

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<sup>1</sup>This is unfortunately the appellation used by physicists, which differ from what I termed theory in section 2.1. Throughout the present chapter theory is not used in the sense of this section.

of Domb. In fact, Widom, being a chemist, came from another part of science than the mathematically trained Domb.

Before enunciating Widom's work, let us look at how he got interested in these phenomena. Widom (b. 1927) has offered recollections of his career in an interview with the Physics of Scales group.<sup>2</sup> After graduation from the chemistry department of Columbia University in 1949, he enrolled as a physical chemistry graduate student at Cornell University. His decision to do a theoretical dissertation gave him the choice between either statistical mechanics or quantum mechanics. He chose the latter and worked with Simon Bauer on energy transfer in molecular collisions. During his doctoral studies most of his coursework was in physics (including one on statistical mechanics) and mathematics, which was a "little unusual" at Cornell, "but not unprecedented." Nor was it atypical for chemistry students, even for those doing experimental work, that he did not take any laboratory courses. After finishing his doctoral studies at Cornell in 1952 (degree awarded in 1953), he became a research associate at the department of chemistry of University of North Carolina until 1954. Here he worked with the physical chemist Oscar K. Rice, who examined phase equilibrium and critical points. It was not until then that Widom "really learned phase transition theory and got to appreciate thermodynamics and statistical mechanics" more than he had done at Cornell. To the extent that his work in the 1950s dealt with statistical mechanical models it was more of the Mayer model type than models similar to the lattice gas model. In 1954 he returned to Cornell for good, first as an instructor, but from 1963 as a full professor of chemistry.

Turning to the four papers, one dealt with surface tension at the critical point, whereas the three others concerned relations between critical exponents. Widom put forward several hypotheses culminating with the proposal of his famous scaling hypothesis,<sup>3</sup> which were not derived from microscopic models, but were of macroscopic nature, so they are not relevant in themselves for the issue of this dissertation. However, Widom used the two- and three-dimensional lattice gas model to examine the validity of his hypotheses and this use is what I intend to analyse. Since their publication span is so short, I shall consider the four papers together.

Structurally speaking, the critical values of the lattice gas model played mainly the same role as experimental data, but how did Widom perceive the model? He wrote:

Many of the properties of *true* two- and three dimensional fluids are also known, either theoretically or experimentally. The *true* one-dimensional system, while completely understood, are of no interest here because they do not undergo phase transitions. (Widom; 1962, p. 2803, my emphasis)

Since the only known theoretical properties about fluids concern the lattice gas model, the predicate "true" must apply to this model. On the other hand, in a paper from 1965 he opened for the possibility that a discrepancy between values for this model and a certain hypothesis of his was "due to a significant difference between the lattice-gas model and a continuum fluid[...]."<sup>4</sup> By the latter he meant a real liquid, so it seems like he had not completely settled the issue of the realism of the lattice-gas model.

At any rate, he used the model both to support some hypotheses and to reject others.

<sup>2</sup>Available at the web page of the group: <http://hrst.mit.edu/hrs/renormalization/Widom/index.htm>. Widom's quotations in the following are taking from the interview at this web page.

<sup>3</sup>In Widom (1965a).

<sup>4</sup>Widom (1964).

The paper on the surface tension of liquids<sup>5</sup> contains a spectacular example of both. He reformulated an earlier theory of interfacial tension for a fluid in the neighbourhood of the critical point (the theory was originally proposed by van der Waals and later elaborated by J. W. Cahn and J. E. Hilliard). The result Widom called the square gradient theory. We are neither concerned with the details of this theory nor with the details of Widom's arguments but only with how Widom argued by means of the lattice gas model.

From his reformulation, Widom obtained a relation between critical exponents. Suppose  $L$  is the length of the interface between the liquid and gas phases,  $\gamma$  is the surface tension, and the temperature dependence near the critical point of these two quantities is given by the critical exponents  $\nu$  and  $\mu$ , i.e.  $L \sim |T - T_c|^{-\nu}$ ,  $\gamma \sim |T - T_c|^\mu$ . Using a macroscopic hypothesis which he had previously advocated for, Widom related  $\nu$  and  $\mu$  to other exponents. This meant that the value of an exponent could be obtained, given the values of the other exponents. Now in the cases where *all* the values of the exponents are available, it is possible to check whether they fulfil the relation. Thus, the validity of the relation could be tested and with it the reformulated theory (assuming the validity of the macroscopic hypothesis).

Widom tested the relation in three cases: 1) values of real three-dimensional systems from an analysis of experimental data of inert gases; 2) values of the three-dimensional lattice gas model from accurate numerical estimates; and 3) exact values for the two-dimensional lattice gas model. He concluded that had the results "[...] for the three-dimensional cases [i.e. 1 and 2 above] been previously known they would have been counted outstanding successes of the square-gradient theory."<sup>6</sup> This he based on the agreement between the values of the calculated and the measured exponents for the real fluid, and two independent estimates of  $\nu$  for the three-dimensional lattice gas model (even though the latter was just outside the limits of certainty<sup>7</sup>). This means that not only experimental results for real three dimensional fluids, but also results for the three-dimensional lattice gas model would have counted in favour of the square gradient theory. In other words, the lattice gas model is discussed on par with experimental results.

Widom also used the lattice gas model to argue that the square gradient theory cannot be true, despite its apparent success: The relation predicted by the square gradient theory is not fulfilled for the two-dimensional lattice gas model, so, Widom argued, the theory cannot be correct. In this case, Widom relied only on the lattice gas model without invoking experimental results, even though he expressed uncertainty about the agreement between the lattice gas model and real fluids. Equally interesting is the fact that it was results for the *two*-dimensional model he used. Is it obvious that the two-dimensional model can say anything significant about real systems? Widom seems to have thought so.

At any rate, Widom used the discrepancy to justify a rejection of the square gradient theory and propose a new theory. As a proof of the value he ascribed to the lattice gas model, he once again placed the model on par with experiments: "The resulting theory is in accord with all the facts which are rigorously known analytically, numerically, or experimentally about interfacial tensions and correlation lengths in fluid systems of two or three dimensions."<sup>8</sup> So, Widom used the lattice gas model to both falsify some theories and verify others.

Widom was not the only one who used the model to shoot down theories. Another

<sup>5</sup>Widom (1965b).

<sup>6</sup>Widom (1965b), p. 3895.

<sup>7</sup>Widom (1965b), pp. 3895-6.

<sup>8</sup>Widom (1965b), p. 3893.



example is Michael E. Fisher's use of the model in relation to the scattering of light at the critical point. Since Fisher is one of the protagonists in what follows, it is worthwhile to take a brief look at his biography. Where did Fisher (b. 1931) get his interest in these phenomena from? Probably from Cyril Domb (who has offered some recollections, on which the following is based, of Fisher's early career<sup>9</sup>). Fisher received both his undergraduate and graduate training at the Physics Department at King's College, London (where Domb was teaching). Fisher enrolled here in 1948 and graduated three years later. After two years of national service he returned to the department and began doctoral studies under the supervision of Donald MacKay.<sup>10</sup> The Ph.D. degree was awarded in 1957 for a thesis entitled "The Solution of Problems in Theoretical Physics by Electronic Analogue Methods." Fisher published several papers on the solutions of various differential and integral equations arising in mathematical physics by such methods in the 1950s. In parallel with this preoccupation with the mathematical aspects of theoretical physics, Fisher got interested in statistical mechanics. According to Cyril Domb (1991) the story goes like this. The inaugural lecture by Domb at King's College in 1955 on problems of statistical mechanics combined with Domb's pessimistic view on the prospects of analogue computing, convinced Fisher that it might be worthwhile to work on statistical mechanics instead. Subsequently, Domb and Fisher decided to investigate polyelectrolyte molecules in solutions. However, they collaborated on other subjects as well and wrote a paper on random walks together. I believe it is fair to say that Domb and Fisher were both more interested in the mathematical aspects of the modelling than was the average theoretical physicist. For instance, Domb has said that he "suspect that it was the challenge of exact methods which Michael found particularly attractive."<sup>11</sup> After getting his degree, Fisher continued to work at King's college, where he finally became full professor in 1964. Two years later he left UK for US to take up a position at Cornell. Here he was first a professor of chemistry and mathematics and then of physics and mathematics. In 1987, he exchanged Cornell with the University of Maryland.

Returning to the scattering of light at the critical point, the Ornstein-Zernike theory, which tries to explain critical opalescence – the 'milky' of a liquid at its critical point – on the basis of correlations between densities at different points in the liquid, had been an important theory in this field since its proposal in 1914. However, it could not be tested experimentally as the data were inconclusive.<sup>12</sup> Instead the lattice gas model could be used to raise doubts about the validity of the theory. Fisher wrote that "[a]n obvious defect of the theory can be seen by considering its application to model systems of dimensionality  $d$  different from three."<sup>13</sup> He concluded that for the two dimensional lattice gas model the Ornstein-Zernike theory leads to a clearly unphysical conclusion.<sup>14</sup> This means that the theory "must be suspect for three-dimensional lattice systems."<sup>15</sup> In other words, when the application of the lattice gas model to the Ornstein-Zernike theory led to an unphysical conclusion, this posed a problem for this theory.

<sup>9</sup>Domb (1991).

<sup>10</sup>Domb (1991).

<sup>11</sup>Domb (2003), p. 491.

<sup>12</sup>According to the Physics of Scale homepage, B. Chu provided an experimental refutation of the Ornstein-Zernike theory at the NBS conference in April 1965.

<sup>13</sup>Fisher (1964a), pp. 956-7.

<sup>14</sup>The conclusion is that the correlation function between the densities at two points in the fluid the distance  $r$  apart will vary as  $\log r$  which "is clearly unphysical for large  $r$  and shows that the assumptions of the theory are certainly not to be trusted for two-dimensional systems." Fisher (1964a), p. 957.

<sup>15</sup>Fisher (1964a), p. 957.

The application of models described above diverged from the use around the time of Onsager's solution. Kramers and Wannier and Onsager used the model to show that a mathematically rigorous analysis of a statistical mechanical model can in fact lead to a phase transition. Onsager's analysis of the model was also used to prove that approximations are incorrect. When applied to the Lenz-Ising model, they predict a behaviour of the model which disagrees qualitatively with Onsager's solution for the two-dimensional case. Since Onsager's solution was known to be rigorous, the approximation methods must be wrong. The role played by the lattice gas model in Widom's and Fisher's arguments were of another kind. Here a relation for *real* systems was tested on results for the lattice gas model and these results played a role analogous to experimental data.

## 10.2 Uses of the Lenz-Ising Model to Obtain Understanding

The uses of lattice gas model outlined in the previous section were largely destructive, i.e., they helped to shoot down ideas and theories. However, the Lenz-Ising model was also used in more constructive ways to obtain insight into real systems.

As noted in Chapter 8, C. N. Yang and his brother C. P. Yang compared the lattice gas model with the results of Voronel' and co-workers.<sup>16</sup> From this successful comparison, they drew an interesting conclusion and their paper contains one of the first uses of the model to gain insight into real systems. After having concluded that the model yields a fair qualitative description of the critical point of argon, they connected the behaviour of real physical systems to that of the model:

Now the critical phenomenon of a lattice gas originates from a rapidly changing balance in the competition between the occupied and unoccupied sites. One is thus led to the suggestion that in real gases, the critical phenomenon originates from a rapidly changing balance in the competition between holes and occupied volume. (Yang and Yang; 1964, p. 304)

In other words, they thought that the lattice gas model might qualitatively explain the origin of critical behaviour – that is, a feature found in the model might be transferable to the real gas. Only if the model is believed to capture the essential feature of the physical phenomenon are conclusions about the model transferable to conclusions about the real system. So, such a transfer requires a fundamental confidence in the validity of the model. Obviously, Yang and Yang had this confidence in the lattice gas model.

Simultaneously, Fisher also used the Lenz-Ising model to provide information about real systems, but in a qualitatively different way. He first applied the model to say something about the analogies between real systems. In the 1960s it was realised that a number of critical exponents of disparate physical systems quite precisely have the same experimental values. For instance, in a number of systems an exponent of roughly  $1/3$  appeared: Already in 1945, Guggenheim<sup>17</sup> compiled experimental results for the coexistence curves for a number of fluids in the same graph, showing that they follow a power law with an exponent of roughly  $1/3$ . Remarkably, the same exponent is found for the coexistence curve for the binary system perfluoromethylcyclohexane in carbon tetrachloride and for the magnetisation of the ferromagnet EuS.<sup>18</sup> Such agreements are not only a numero-

<sup>16</sup>Yang and Yang (1964).

<sup>17</sup>Guggenheim (1945).

<sup>18</sup>Fisher (1965), pp. 16-18.

logical coincidence, Fisher argued, the Lenz-Ising model in its various guises was able to “show theoretically that this analogy, between what are at first sight very different physical systems, is not merely superficial, but can be made quite precise.”<sup>19</sup> Based on the mathematical analogy between the Lenz-Ising model as a representation of a gas and a ferromagnet, respectively, Fisher was able to explain the coincidence of the values for these two physical systems. Fisher continued:

Of course, these relations are only exact for an Ising ferromagnet and a lattice gas. However, in as far as we believe that these models are at all ‘realistic,’ we may now draw the theoretical conclusion that we should *expect* the critical behaviour for gases and ferromagnets to be very similar! In particular, in addition to the correspondence between the spontaneous magnetization and coexistence curves, the divergence of the susceptibility and compressibility, and the specific heat anomalies should match. (Fisher; 1965, p. 34, emphasis in the original)

In this way, the Lenz-Ising model could help explain why we find the same critical behaviour in *real* systems.

The next thing Fisher did was to use his comparison of the model with experiments, already discussed in Chapter 8, to draw some very interesting conclusions regarding the nature of the critical points. The following discussion starts with his analysis of the Heisenberg model rather than the Lenz-Ising model, because he was more explicit here and because his analysis of the Lenz-Ising model draws on the former analysis.

The critical exponent  $\gamma$  characterises the temperature dependence of the ferromagnetic susceptibility. According to Fisher,<sup>20</sup> the best experimental value for this exponent for nickel was obtained by Kouvel and Fisher (1964) from an analysis of the 1926 experimental results of Weiss and Forrer, which yielded  $\gamma_{\text{nickel}} = 1.35 \pm 0.02$ . He compared this value with classical predictions (see section 6.1) and numerical results based on series expansions for the Lenz-Ising model and the Heisenberg model:

This value of  $\gamma$  lies well above, not only its classical prediction, but also above the value  $\gamma = 1.25$  for the three-dimensional Ising model. All the more surprisingly, it agrees closely (to within its theoretical and experimental uncertainties) with the prediction  $\gamma \simeq 4/3$  for the nearest neighbour Heisenberg model! As we explained, it is difficult to believe that the localized spin Heisenberg picture is a realistic model for nickel. (Fisher; 1965, p. 90)

The problem with the fundamental localised spin assumption of the Heisenberg model for nickel is described in section 8.1. Fisher’s conclusion was that the validity of this assumption for this material is not at all certain. He continued the quotation with the words:

We thus seem forced to conclude that the behaviour close to  $T_c$  is *insensitive* to the details of the true Hamiltonian. Only the general statistical features notably the dimensionality and the, presumably, finite ranged and isotropic interactions seem to determine the nature of the singularity. (Fisher; 1965, pp. 90-91, emphasis in the original)

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<sup>19</sup>Fisher (1965), p. 18.

<sup>20</sup>Fisher (1965).

His argumentation in these two quotations is quite interesting. Instead of simply concluding that the agreement between the Heisenberg model and experiments is surprisingly good, he combined this agreement with the model's lack of realism. Since the model is unrealistic for this material, but is capable of describing the experimental data well, it seems natural to believe that it is not the details of the model which determines its critical behaviour. Consequently one is led to conclude that the behaviour of the phenomenon is insensitive to the details.

As regards the Lenz-Ising model, Fisher reached the same conclusion from the same line of argument, this time for the critical exponent  $\beta$  characterising the temperature dependence of the magnetisation. From series expansions studies of the three dimensional model, he concluded that  $\beta \cong 5/16 = 0.3125$ . It is surprising, he wrote, "that such a simplified model of a magnet or a gas could lead to a result for the exponent  $\beta$  so close to the experimentally observed one third laws."<sup>21</sup> In an echo of the arguments concerning the Heisenberg model above, he continued: "Again the conclusion is forced on us that the detailed properties of the Hamiltonian become relatively unimportant in the critical region, whereas the dimensionality becomes a prime factor."<sup>22</sup> He illustrated this by appealing to the graph by Burley (1960) (reproduced on figure 7.1) depicting the magnetisation of the two and three-dimensional Lenz-Ising model as a function of temperature for various lattices. The figure shows clearly that the differences between the two dimensions are much larger than between the various lattice structures for a single dimension.

Fisher had to assume that the Lenz-Ising model is not completely removed from real systems, because then it would have no chance of saying anything important about such systems. This means that this model has the right balance between realism and unrealism so that it is possible to conclude something about the behaviour of real physical systems from the agreement between the model and experimental data. Fisher used precisely the unrealism of the model as a lever to obtain insight into real phenomena. If the model had been more realistic it would not have been possible to obtain this insight because then the agreement would not have been a mystery: it is no wonder that a realistic model is empirically adequate. Not in spite of the lack of realism of the Lenz-Ising model but *because* of it, Fisher was able to argue for one of the most important insight in the area of critical phenomena, namely that their behaviour is insensitive to the details of their constituents. This new use of the Lenz-Ising model broke radically with the previous uses – both the ones of the 1950s, but also that of Widom.

Could Fisher have reached this conclusion without reference to either experiments or models? If precise measurements of the critical properties of a host of different magnetic materials with a range of different spin conditions had been available, it might have been possible to draw the same conclusion. However, such measurements were not present. In principle, he could have reached the same conclusion from considerations on models alone if it had been possible to manipulate *realistic* models. However, this would require the manipulation of sufficiently realistic models which mimic real materials at one's will and this was far from possible.

Despite the good agreement between the theoretical and the experimental  $\beta$ , there is also a discrepancy: "The artificial nature of the Ising model does therefore make itself felt, but [...] to a much smaller extent than might have been guessed."<sup>23</sup> This led Fisher to some considerations about the "theoretical task", namely "to characterize just

<sup>21</sup>Fisher (1965), p. 106.

<sup>22</sup>Fisher (1965), p. 106.

<sup>23</sup>Fisher (1965), p. 106.

which *relevant* features of real systems are oversimplified by the model.” (Emphasis in the original)<sup>24</sup> One way to examine which of the relevant features are oversimplified by the Lenz-Ising model is to compare it with the Heisenberg model. However, since several of the relevant critical exponents could not be obtained for the Heisenberg model, such an examination was not feasible.<sup>25</sup>

In sum, a shift in the epistemological status of the Lenz-Ising model occurred during the 1960s. Before, Kramers, Wannier and Onsager considered the Lenz-Ising model to be a step towards an understanding of cooperative phenomena. However, in a sense the understanding was only negative: the Lenz-Ising model could say something about the mathematical aspects of phase transition, but not anything positive about real systems because the model was considered to be too far removed from real systems. In addition to stressing this ‘distance’ from real systems, they did not find it worthwhile to compare their theoretical results for the model with experimental results. In contrast, in the 1960s the model was actually found to give insight into real systems. I propose to make a fundamental distinction between constructive and destructive uses of models in general and the Lenz-Ising model in particular. The destructive use is the one applied by Widom (and Fisher for the Ornstein-Zernike theory) where hypotheses or theories are shot down. Fisher (and the Yang brothers) used the model to say something positive about the behaviour of real systems. Fisher used the model to distinguish essential from inessential features of the real system. However, a systematic use of simple models within the field of critical phenomena first occurred in the second half of the decade. I shall now turn to this.

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<sup>24</sup>Fisher (1965), p. 106.

<sup>25</sup>In fact, Fisher was pessimistic about the prospects of determining the value of  $\beta$  for the Heisenberg model:

Unfortunately, there seems no way at present in which one might seek to estimate  $\beta$  for the Heisenberg model. The low-temperature behaviour in that case is given by the spin wave expansion and its correction terms which have proved exceedingly difficult to calculate. There are, however, good reasons for believing that the spin wave approach yields only an asymptotic series (terms like  $e^{-J/kT}$  are neglected) so that even the complete series might not describe the critical point behaviour. (Fisher; 1965, p. 106)

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## The Role of the Lenz-Ising Model 1965-1970: Theory Function

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The previous chapter described how the Lenz-Ising model was used to perform specific tasks in the first half of the 1960s, for instance to test the validity of various hypotheses about real systems. In the last half of the 1960s the Lenz-Ising model, along with similar ‘simple’ models, was put to a more systematic use in order to gain insight into critical phenomena in general. To borrow a term from the title of a review paper by Michael E. Fisher,<sup>1</sup> a *theory* of critical phenomena appeared in the 1960s (here ‘theory’ is used in the sense of section 2.1). The use of the Lenz-Ising model in the endeavour to create a theory is the subject of the present chapter. In addition, the chapter will document that in the 1960s the Lenz-Ising model provided a model universe which was used to gain insight into real systems.

This focus on the theory of critical phenomena means that the chapter will not treat the host of more specific tasks performed by the Lenz-Ising model in the massive literature on this model in the 1960s (see Appendix A). Many of these papers present new results about the model, but the model is rarely placed in the larger modelling context. Consequently they cannot be used to examine the role of the model in this larger framework. Review articles and books or chapters aimed at novices in the field are much better suited for this task, so the following discussion is mainly restricted to such contributions (even though there are a few detours to the original research literature). In accordance with this choice, I shall base my deliberations on a review paper (the influential one by Fisher mentioned above) and a textbook of 1971 (by H. Eugene Stanley,<sup>2</sup>) but I shall use other sources as well to document the generality of these two accounts.

I do not want to claim that the following discussion of the role played by the Lenz-Ising model is complete, and the model was undoubtedly used in several other ways. Moreover, the views which will be presented are not representative for all those who worked in the field. However, I do believe that the materials used, which arguably are among the most influential of their time, do represent an important movement of which many of Fisher and Stanley’s contemporaries would consider themselves as members.

A reader familiar with the development of critical phenomena in the 1960s, will perhaps be surprised by the absence here of some of the most important developments in critical phenomena in this decade, such as the scaling hypothesis (of Widom, Hunter and Domb, Patashinskii and Pokrovskii, and Kadanoff) and the block spin approach of Kadanoff.<sup>3</sup> These developments are absent, not because I find them insignificant, nor because the Lenz-Ising model did not play a role in them, but because the chapter is aimed at giving an overview of the role played by the Lenz-Ising model in the *theory* of critical

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<sup>1</sup>Fisher (1967).

<sup>2</sup>Stanley (1971).

<sup>3</sup>See Domb (1996), pp. 219-238.

phenomena more generally. The role played within these specific developments is similar to the one described in the preceding chapter, whereas the model played a novel role within the theory described in this chapter.

## 11.1 Critical Phenomena

In order to examine the role played by the Lenz-Ising model to get insight into critical phenomena, it is necessary to take a brief look at this field in the 1960s. More precisely we have to answer two questions: 1) What aspects of critical phenomena were found to be in need of understanding? 2) And how was this understanding to be achieved? This section answers the first question, while the next one deals with the second question.

Mainly due to new experimental results, but also to theoretical developments, it was gradually realised in the first half of the 1960s, that time was ripe for a general understanding of critical phenomena.<sup>4</sup> As pointed out by Steven G. Brush in several places<sup>5</sup> and by Hoddeson, Shubert, Heims and Baym (1992) (and passed on in Part One of this dissertation), it was well-known at least since the early 1940s that numerous physically disparate phenomena displayed analogous behaviour; most importantly they all have a transition point. However, in the 1960s a subclass of these phenomena was singled out, namely critical phenomena. To these phenomena belong what I have called the four core areas: the critical point of the liquid-gas transition, the Curie point of ferromagnets, the Néel point of antiferromagnets and the order-disorder transition in binary alloys. In the 1960s it was realised that critical phenomena not only have qualitative features in common but also share (at least roughly) the same values of critical exponents.

A seminal conference on ‘Phenomena in the neighborhood of critical points’ was held at the National Bureau of Standards, Washington (D.C.) in April 1965. In the introduction to the proceedings, the chairman M. S. Green recapitulated some recent scientific developments which “contributed to the feeling on the part of a number of scientists, and in particular, on the part of those who formed themselves into an *ad hoc* committee to organize it [the conference], that April 1965 was an appropriate moment for a conference on critical phenomena.”<sup>6</sup> Green mentioned four such developments: 1) The theoretical result that the three-dimensional Lenz-Ising model exhibits non-classical critical behaviour. Two sorts of treatments give rise to classical<sup>7</sup> behaviour: Mean-field theories such as van der Waals for gases and thermodynamical theories assuming that the free energy can be Taylor expanded (see section 6.1). 2) Voronel’ and collaborators’ experimental evidence that the specific heat of argon, respectively oxygen has a singularity at the transition point, which is very similar to the one found for the  $\lambda$  transition in liquid helium. 3) The experimental finding that the curve of the magnetisation as function of temperature for ferromagnets and antiferromagnets has a shape similar to the coexistence curve of the liquid-gas. Moreover, that the shape of analogous quantities for the three-dimensional Lenz-Ising model is similar to these curves. 4) The theoretical objections to the classical Ornstein-Zernike theory raised by Fisher (mentioned on page 142) and others, as well as experimental deviations from this theory.

The conference marked the emergence of the view that a theory of critical phenomena

<sup>4</sup>Green (1966).

<sup>5</sup>See Brush (1983).

<sup>6</sup>Green (1966), p. xi.

<sup>7</sup>Classical here means standard, well-known.

should deal especially with two points. The first is described nicely by Michael E. Fisher in the review paper from 1967:

Consequently a problem of central interest in the study of critical phenomena, both experimentally and theoretically, is the determination of the asymptotic laws governing the approach to a critical point [...] Theories competent to make significant predictions about critical-point behaviour have, however, developed mainly in the past decade or two and have been a focal point of activity in the last few years. (Fisher; 1967, pp. 617-8)

This behaviour was typically described in terms of critical point exponents, which were of central importance for the theory. For critical exponents the precise values of a range of parameters which are specific to each system are insignificant. For instance, the critical temperature can vary from one system to the next by up to six orders of magnitude,<sup>8</sup> but it is irrelevant for the value of the critical exponent; what matters is overall features of the behaviour and this is epitomised in the critical exponents. The justification for focusing on the critical exponent rather than the entire function was that it was often found experimentally that the corresponding term dominates near the critical point.<sup>9</sup>

In fact, this similarities between different systems was the second point of central importance and at the conference these similarities really came to the fore. In his introduction mentioned above, Green concluded that the pertinent questions at the conference could be summarised into two questions: are the phenomena really analogous and what do they share which can account for the singular behaviour of their analogous properties.<sup>10</sup>

After the conference the determination of the exponents and the understanding of the universal but non-classical behaviour, to use Uhlenbeck's expression at conference,<sup>11</sup> became the central problems. Leo P. Kadanoff at the University of Illinois and his group stated in a review paper of 1967 what they considered to be the central question: "This simplicity and similarity among phase transitions is not fully elucidated theoretically. Some of the qualitative features of this behaviour are reasonably well understood; others remain a complete mystery."<sup>12</sup> The particular subject of their paper was "what can be learned by comparing different phase transitions with each other and with the existing theories. How are different phase transitions alike? In what ways do they differ? Why should we expect these similarities and differences?"<sup>13</sup>

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<sup>8</sup>Stanley (1999), p. S364.

<sup>9</sup>See Stanley (1971), p. 40.

<sup>10</sup>See Green (1966), p. xi.

<sup>11</sup>Uhlenbeck (1966).

<sup>12</sup>Kadanoff et al. (1967), p. 395.

<sup>13</sup>Kadanoff et al. (1967), p. 395. Stanley et al. (1971), in a paper at the Enrico Fermi International School of Physics, wrote:

In recent years considerable experimental and theoretical attention has been directed toward the study of critical point exponents. Very recently increasing attention has been focused on the question of precisely which features of a physical system are relevant for determining the critical point exponents and which are not relevant. (Stanley et al.; 1971, p. 246)



## 11.2 Fisher's Programme

These were the problems, but how could and should they be solved? In the review paper by Fisher mentioned above, he found it necessary to give an explicit exposition of the main aim of theory<sup>14</sup> and he stated his approach in opposition to what he called the traditional approach: "This is sometimes held (implicitly or explicitly) to be the calculation of the observable properties of a system from first principles using the full microscopic quantum-mechanical description of the constituent electrons, protons and neutrons."<sup>15</sup> After the Hamiltonian of these constituents is established, it is approximated and one attempts to find the eigenstates, the energy levels etc. by running Schrödinger's equation.<sup>16</sup> This approach, which is often the one taken in quantum chemistry, is rarely feasible for the complicated systems of condensed matter physics. Moreover, Fisher claimed "it is not even a very sensible one!"<sup>17</sup> He gave the following reason in 1983:

The modern attitude is, rather, that the task of the theorist is to *understand* what is going on and to elucidate which are the crucial features of the problem. For instance, if it is asserted that the exponent  $\alpha$  depends on the dimensionality,  $d$ , and on the symmetry number,  $n$ , but not on other factors, then the theorist's job is to explain *why* this is so and subject to what provisos. If one had a large enough computer to solve Schrödinger's equation and the answers came out that way, one would still have *no understanding* of why this was the case! Thus the need is to gain understanding, not just numerical answers: that does not necessarily mean going back to Schrödinger's equation which, in any case, should be really regarded just as an approximation to some sort of gauge field theory. (Fisher; 1983, p. 46, emphasis in the original)

In the paper of 1967, he wrote what should be done instead:

[...] the aim of the theory of a complex phenomenon should be to elucidate which features of the Hamiltonian of the system would lead to the most characteristic and typical observed properties. Initially one should aim at a broad qualitative understanding, successively refining one's quantitative grasp of the problem when it becomes clear that the main features have been found. (Fisher; 1967, p. 619)

This view of the aim of theory and the main steps in its development I call *Fisher's programme*. The fulfilment of this programme requires extensive use of simple models like the Lenz-Ising model:

To achieve these ends the study of 'model systems' has been increasingly rewarding. The ideal model should provide as realistic a description as possible of those features of a physical system believed to be important for the phenomena under study but, at the same time, should be tractable mathematically. Without this second characteristic, theoretical discussion frequently

<sup>14</sup>In fact, he did this in the three reviews papers: Fisher (1965), Fisher (1967), and Fisher (1983). They all express roughly the same view and consequently I will not treat each of them individually.

<sup>15</sup>Fisher (1967), p. 619.

<sup>16</sup>Fisher (1983), p. 46.

<sup>17</sup>Fisher (1983), p. 46.

adds little more to one's understanding than that gained directly from experiments. Conversely one should always attempt to refine a model in order to test how far its defects as a true microscopic description affect the conclusion drawn. (Fisher; 1967, p. 619)

Fisher added a footnote: "The philosophy advanced here has been vividly expounded by Frenkel" in 1946.<sup>18</sup> In order to examine which features are relevant and which are irrelevant, one should employ numerous models and not concentrate on a single one.<sup>19</sup>

To sum up, Fisher's characterisation of the new approach contains four important components:

- The theorists seek not only explanation in the sense of reproduction of important features of a particular real system, but understanding of the system in question and the mechanisms responsible for these features.
- More precisely, in Fisher's sense of the word, understanding means to shed light on which properties of the Hamiltonian of the system lead to the characteristic and typically observed properties of the system.
- This perception of understanding has consequences for the methodology of investigation: Due to the mathematical intricacies of realistic model systems one should look at caricature models, which were described on page 20. Such models focus on a few features of the system, rather than on all its peculiarities.
- To distinguish the essential from the inessential features, a range of models rather a single one should be considered and examined.

Fisher argued that the preceding development within critical phenomena had, in fact, followed this route:

The recent history of the study of critical phenomena has, in the main, followed the course of simplifying the physical models while improving and strengthening the mathematical techniques to the stage where, at last, fairly accurate theoretical treatments can be given for models which, while gross oversimplifications of reality in many respects, do certainly embody a number of the vital features of the particles and interactions leading to phase transitions and critical points. (Fisher; 1967, p. 619-20)

Fisher's attitude toward the role of models was linked with a vision about what it means to understand physical phenomena and how they should be modelled. A discussion of this important issue is postponed to Chapter 12. This chapter also discusses the correctness of Fisher's description of the traditional approach to modelling.

If Fisher's programme is construed generally enough, which does not seem unreasonable, namely as aiming at uncovering what features of the Hamiltonian lead to what kind of behaviour at the critical point, then it was endorsed by several scientists. For instance, even though Kadanoff and collaborators did not explicitly subscribe to Fisher's programme in their review paper,<sup>20</sup> in reality they did follow it. Moreover, in his textbook, Stanley subscribed to this program and pointed out how it should be accomplished:<sup>21</sup>

<sup>18</sup>Fisher (1967), p. 619.

<sup>19</sup>Fisher (1983), p. 47.

<sup>20</sup>Kadanoff et al. (1967).

<sup>21</sup>In fact, Stanley wrote that a fulfilment of his goal above would not be enough:

Certainly a first goal of any theory of critical phenomena is to find such theoretical models [such as the three-dimensional Lenz-Ising and Heisenberg model] and, moreover, to understand which features of the models are relevant in determining the values of the critical-point exponents and which are not. (Stanley; 1971, p. 49)

Not every scientist working on critical phenomena in the 1960s would subscribe to Fisher's programme; some researchers, such as Joseph E. Mayer, concentrated on the critical point of liquids alone and showed no interest in critical phenomena in general. Consequently, they probably did not see their work as contributing to this programme. However, it is possible to single out a substantial group of researchers who were all committed to Fisher's programme.

The statements about the aim of theory in this section are to be understood as declarations of intent. How Fisher's programme was pursued and the role played by the Lenz-Ising model are the topics of the next sections.

### 11.3 Fisher's Review Paper

Fisher's review paper of 1967 was not devoted exclusively to his own programme. It was primarily a status report on the state and situation of critical phenomena at the time of writing. Based on a section of his entitled 'Conclusion and Outlook,' where Fisher stated both what he found had been done and what needed to be done, I shall analyse the role played by the Lenz-Ising model in the partial accomplishment of the programme present in the paper.

Some of the results behind Fisher's conclusions were well known prior to 1967 and have already been discussed in the preceding chapter. However, Fisher used this material in a new and more systematic way, which sheds light on how he thought his programme ought to be accomplished. Of central interest to Fisher was the perhaps most fundamental result concerning the Lenz-Ising model, both the two and three-dimensional variants, viz. the strong influence of dimension on critical behaviour. It was well known already in the early 1960s that for a number of critical exponents the *dimensionality* of the lattice on which the model 'lives' is of much greater importance than the type of lattice. At the time of Fisher's review these tentative conclusions had gained corroboration and he could conclude that for the Lenz-Ising model, both the two and three-dimensional variants, "[t]he strong influence of dimensionality has been clearly demonstrated[...]."<sup>22</sup> Fisher found this result to be of great importance. I shortly shall discuss why.

Concerning the state of his programme more generally, Fisher wrote that "The dependence of the critical-point exponents on the Hamiltonian (as well as the dimensionality) is demonstrated by the results for the Heisenberg model."<sup>23</sup> However, "[...] much remains

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Even if we should eventually succeed in this first goal, we will still be left with the question, 'Isn't there some underlying theory of all these exponents which tells us how they hang together?' A second goal, then, is to study relations among the various exponents. (Stanley; 1971, p. 49)

There is no indication that Stanley thought that an answer to this natural question would provide understanding of critical phenomena. Therefore it will not be discussed in relation to Fisher's programme. However, since it was an important question, and microscopic models played a role in its examination, it will be briefly touched upon in a later section.

<sup>22</sup>Fisher (1967), p. 718.

<sup>23</sup>Fisher (1967), p. 719.

to be elucidated and understood,”<sup>24</sup> and Fisher expressed the expectation that future work would clarify the dependence on spin and anisotropy of the interaction. So, in this discussion, Fisher took some steps towards the accomplishment of this programme: It is clear that the dimensionality of the lattice influences the critical exponents considerably, and the spin and the anisotropy of the interaction, too, seem to be important, but further investigations are required. However, he did not point to the need of examining the conclusion for other models than the Lenz-Ising and the Heisenberg models.

The second of the ‘old’ results he put in a new light was the analogies between various systems. Fisher’s use of the Lenz-Ising model in this respect has already been considered in section 10.2. In the review, he repeated the conclusion that the model provide understanding into why various physical systems share roughly the same values of critical exponents; indeed he counted it as one of the “successes of present theory.”<sup>25</sup> Interestingly, there is a similar analogy between the mean-field model of ferromagnetism (the Weiss model) and that of liquid-gases (van der Waals). However, Fisher and most of his contemporaries did not think that this analogy provide the same understanding of similarity of the two types of phenomena. It is reasonable to assume that the lack of realism of the mean-field model was the cause of this model’s lack of explanatory power. If this is correct then the Lenz-Ising model was important because it stroke the right balance between realism and tractability: it was possible to examine the model and at the same time, the model is close enough to real systems that the conclusions drawn about the model have a bearing on real systems. The equivalence of the various guises of the Lenz-Ising model could also help to accomplish Fisher’s programme: “[...] the way is open to understand the often relatively small quantitative differences of behaviour [of the disparate physical systems] in terms of essential differences in the Hamiltonians.”<sup>26</sup> So, once again the Lenz-Ising model could be used to gain understanding. In fact, it played a prominent role in this respect.

The third and final of the ‘old’ results which Fisher placed in a new light was the argument that the Lenz-Ising model reveals the invalidity of the ‘classical’ theories (see 6.1). As previously, the conclusion was that the two- and three-dimensional Lenz-Ising models “definitely establish that the classical conclusions are generally untenable.”<sup>27</sup> Moreover, in the conclusion, Fisher wrote: “The defects of the classical treatments (and their limiting validity) have been thoroughly revealed and understood theoretically.”<sup>28</sup> For instance, the Lenz-Ising model could be used to argue that the classical theories are valid when the dimensionality  $d$  of the lattice becomes infinite. This had not been rigorously established, but “one convincing piece of evidence” is an expansion by Fisher and Gaunt of 1965 of the critical temperature  $T_c(d)$  for a  $d$ -dimensional hyper-cubic lattice. They found the following ratio between this temperature and that of the mean-field model,  $T_c^{\text{mean-field}}$ :

$$\frac{T_c(d)}{T_c^{\text{mean-field}}} = 1 - (2d)^{-1} - \frac{1}{3}(2d)^{-2} \dots \quad (11.1)$$

So in the limit of  $d$  the critical temperature approaches the mean-field temperature and it was thought that in this limit the Lenz-Ising model behaves like the mean-field model. In other words, the Lenz-Ising model could be used to understand both precisely where the classical theories break down, but also why they yield critical exponents which, while not

<sup>24</sup>Fisher (1967), p. 719.

<sup>25</sup>Fisher (1967), p. 718.

<sup>26</sup>Fisher (1967), p. 718.

<sup>27</sup>Fisher (1967), pp. 662-3.

<sup>28</sup>Fisher (1967), p. 718.

exactly correct, are not far from the correct values. The explanation is of course somewhat abstract: they become exact in the limit of infinite dimension (which is physically unrealistic). Instead of being content with the conclusion that the classical theories are unable to describe real systems and then move on to more promising approaches, Fisher (and others) wanted to understand *why* this is the case and to what extent these theories are valid.

The analysis above shows that Fisher used the Lenz-Ising model extensively, and to a lesser extent the Heisenberg model, to accomplish his programme. In his discussion of what features of the Hamiltonian give rise to what critical behaviour, he mentioned lattice dimensionality, spin dimensionality and anisotropy of interaction. Judging from this discussion, these were the important features to consider.

He wrote about the possibility of furnishing further insight:

To go forward it is now also necessary to calculate [critical exponents] reliably for somewhat more realistic models. It seems premature to hope for rapid progress on the continuum-gas models in the critical region, although the deviations of the observed critical exponents from lattice-gas results make this very desirable. As a first step, lattice gases with hard cores of larger sizes (relative to the lattice spacing) as well as attractive interactions might well be studied [...] (Fisher; 1967, p. 719)

Fisher also advocated the examination of more realistic models of magnetism.<sup>29</sup> However, at the same time he advised to go in the opposite direction as well:

[...] less realistic, but mathematically more tractable, models should still be devised and pursued since their properties, if accurately determined, will doubtless be useful in deepening our understanding of the interplay between dimensionality and the specific features of the model Hamiltonian even if these are not too realistic. (Fisher; 1967, p. 719)

The notion of understanding employed by Fisher was quite general and abstract.

One aspect of his conclusions seems worthy of attention, namely the dimensionality of the lattice: Why this obsession with the dimension of the lattice when most physical systems are three-dimensional? Or more precisely, what kind of insight did Fisher think that the dimensionality dependence would give? Since Onsager's proof in 1944, it was known that the one-dimensional Lenz-Ising model do not display a phase transition, whereas the higher dimensional variants do. This result demonstrates clearly the importance of the dimension for critical phenomena. However, would an examination of the dependence of critical behaviour on dimension give insight into real systems? In a paper, mentioned above in relation to the validity of mean-field theory, Fisher and Gaunt examined the Lenz-Ising model for lattices of dimensions higher than three. About their motivation they wrote:

Of course the behavior of model physical systems in four or more space-like dimensions is not directly relevant to comparison with experiment! We can hope, however, to gain theoretical insight into the general mechanism and nature of phase transitions. (Fisher and Gaunt; 1964, p. A225)

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<sup>29</sup>See Fisher (1967), p. 719.

Unfortunately, they did not elaborate on what kind of insight such an investigation might yield. Was it because some real systems can be perceived as being of dimension less than three and Fisher and collaborators wanted to see whether the differences between real systems of different dimension were reflected in the models? However, as in the 1950s, where the only real system of dimension lower than three known to exhibit a phase transition was adsorption on a surface, in the 1960s no one-dimensional and only a few two-dimensional systems were discussed in relation to critical phenomena (this was before the age of magnetic films). For instance, Fisher (1967) wrote about Onsager's and Yang's result on the exponent  $\beta$  of the coexistence curve of the two-dimensional Lenz-Ising model: "In principle the result  $\beta = 1/8$  could be tested on real "two-dimensional" systems, notably *adsorbed monolayers*." (Emphasis in the original.)<sup>30</sup> However, he continued, even though experimental data were available this seems not to have been done (Fisher did not himself undertake such a test). Moreover, Fisher expressed the view that the importance of the two-dimensional results was the light they shed, not on real two-dimensional system, but on the classical theories and on the features of *three*-dimensional systems.<sup>31</sup> In order to explore how systems of dimension lower than three are thought to provide insight into our three-dimensional world, we can turn to the treatment of one-dimensional systems in a monograph by Lieb and Mattis entitled 'Mathematical Physics in One Dimension' of 1966:

[...] for a long time it was thought that the physical explanation of ferromagnetism was as follows: electrons interact with their nearest neighbours by means of an 'exchange integral' which tends to line up their spins. This problem we considered in one dimension [...] and it was found that these exchange corrections notwithstanding, the ground state of interacting electrons was always *nonmagnetic*. Therefore the ferromagnetism of real materials (iron, nickel, gadolinium, etc.) must be due to the three-dimensional structure of space, which is responsible for orbital degeneracy, Hund's rules for magnetic atoms, etc. Thus the study of a one-dimensional model pinpointed the probable cause of ferromagnetism in three dimensions. (Lieb and Mattis; 1966, p. vi)

So, according to Lieb and Mattis the one-dimensional system did in fact reveal information about which aspects of a phenomenon can be ascribed to the dimension of the system and which are the same for all dimensions. It is not unreasonable to assume that this explanation carries over to Fisher's interest in dimensionality in his programme. If this is the case, it reveals something quite characteristic of this programme: the approach is to vary the features in all sorts of respects and see how this affects the behaviour of the system. This will, hopefully, give insight into both the essential and the inessential features of the real system.

<sup>30</sup>Fisher (1965), p. 61.

<sup>31</sup>Another example can be found in magnetism. According to Bonner and Fisher (1964), it was realized in the late 1950s-early 1960s that in some crystals (e.g., copper tetramine sulfate monohydrate) the magnetic ions are arranged in chains with strong interaction along the extension of the chain, but quite weak interchain interaction. So, the magnetic behaviour of such crystal should be well represented by a one-dimensional model. However, there seems to be agreement that the main importance of dimensions should not be found in such properties of a small number of materials.

## 11.4 Stanley's textbook

The textbook quality of Stanley's influential monograph on phase transitions and critical phenomena of 1971<sup>32</sup> makes it reasonable to assume that the views it expressed were not only idiosyncrasies held by the author but were prevalent in the community. This is the reason for taking up this monograph here.

As already shown above, Stanley here subscribed to Fisher's programme. The title of his dissertation of 1967 at Harvard, "Critical Phenomena in Heisenberg Models of Magnetism,"<sup>33</sup> reveals his preoccupation with the Heisenberg models, which are general spin models with nearest-neighbour interaction. These models were the subject of a series of papers that he wrote from the middle of the 1960s to the early 1970s. Their overall theme was to determine, in the words of one of the titles, the "[d]ependence of critical properties of Heisenberg magnets upon spin and lattice".<sup>34</sup> In the very early 1970s he turned the issue raised in the above title from a question that was interesting but of limited scope, into a question of central importance for the theory of critical phenomena. In the process the question was changed, in the words of a chapter title<sup>35</sup> to "On what features of an interaction Hamiltonian do critical-points exponents depend?" This question, which fits well into Fisher's programme, was one of the central questions of his textbook.

The aspect of his monograph which concerns us here is the use of a certain class of models. This class included the Lenz-Ising model, but other models as well. In order to appreciate the role played by the Lenz-Ising model in Stanley's textbook it is necessary to discuss his general approach to critical phenomena. One of the most revealing features is his dealing with infinite spin systems, so even though this is not the Lenz-Ising model, it will be given a detailed discussion in the next section.

Turning to the class of models considered by Stanley, their main components are spins which are placed on the sites of a lattice of dimension  $d$  as usual, but they are generalised to be  $D$ -dimensional unit vectors. If  $(S_{i1}, S_{i2}, \dots, S_{iD})$  are the Cartesian coordinates of spin  $\mathbf{S}_i^{(D)}$  then  $\mathbf{S}_i^{(D)} \cdot \mathbf{S}_j^{(D)} = \sum_{n=1}^D S_{in} S_{jn}$  denote the usual scalar product. The model Hamiltonian may be written as

$$\mathcal{H}^{(D)} = -J \sum_{\langle ij \rangle} \mathbf{S}_i^{(D)} \cdot \mathbf{S}_j^{(D)}, \quad (11.2)$$

where the sum is over pairs of nearest neighbours (indicated by the symbol  $\langle ij \rangle$ ).

Depending on the values of  $D$  and  $d$  this equation describes different models; in particular, four models often studied corresponds to four special cases of pairs of  $D$  and  $d$ .<sup>36</sup> Stanley went through the model for different values of  $D$ . For  $D = 1$ , equation (11.2) reduces to the Hamiltonian for the  $d$ -dimensional Lenz-Ising model and Stanley subscribed to the view of the realism of this model held in general in the 1960s.<sup>37</sup> The Hamiltonian

<sup>32</sup>Even though it was published in the year of the advent of Wilson's renormalisation group technique, it did not include a discussion of this topic.

<sup>33</sup>Supervised by T. A. Kaplan and J. H. Van Vleck

<sup>34</sup>One important aspect was whether  $\gamma$ , the critical-point exponent characterising the temperature dependence of the susceptibility, depend on the general spin quantum numbers. In his papers he fluctuated between a "yes" and a "no".

<sup>35</sup>Co-authored with his research students Alexander Hankey and M. Howard Lee.

<sup>36</sup>However, "[m]ore complicated interactions can be taken into account by systematic modifications of this model." (Stanley; 1971, pp. 110-1) Does this mean that he thought that one should continue to make more and more complicated models? Not necessarily. Rather, it is an argument to support the choice of the general Hamiltonian as a good starting point.

<sup>37</sup>He wrote: "Although it was first introduced as a crude model of ferromagnetism, the Ising model has come

D	Hamiltonian	Name	System
1	$\mathcal{H} = -J \sum_{\langle ij \rangle} S_{ix} S_{jx}$	Ising model	one-component fluid; binary alloy, mixture
2	$\mathcal{H} = -J \sum_{\langle ij \rangle} S_{ix} S_{jx} + S_{iy} S_{jy}$	plane rotator model (Vaks Larkin model)	$\lambda$ -transition in a Bose fluid
3	$\mathcal{H} = -J \sum_{\langle ij \rangle} S_{ix} S_{jx} + S_{iy} S_{jy} + S_{iz} S_{jz}$	Classical Heisenberg model	ferromagnet; antiferromagnet
$\vdots$			
$\infty$	$\mathcal{H} = -J \sum_{\langle ij \rangle} (\sum_{n=1}^{\infty} S_{in} S_{jn})$	spherical model	none

**Figure 11.1:** Figure from Stanley (1971) (originally from Stanley and Lee (1971)).

for  $D = 2$  has several names; in addition to the ones used in figure 11.1, the  $XY$  model is widespread. V. G. Vaks and A. I. Larkin used it as a lattice model for the superfluid transition of a Bose fluid.<sup>38</sup> The classical Heisenberg model emerges if  $D = 3$ . For  $D > 3$ , i.e. spins of dimension higher than 3, the system given by equation (11.2) is still well-defined, even though “[...] no physical system has been put forward that corresponds to, say, four-dimensional spins.”<sup>39</sup> This case is mainly examined in the limit  $D \rightarrow \infty$  which has no chance of being realized by a real system. In this limit the model becomes equal to the so-called spherical model of Berlin and Kac. In this model each spin can have any length, but subject to the restriction that the sum of all the spin lengths is equal to the number of spins. This somewhat strange model is also known as the spherical approximation to the Lenz-Ising model and this role was the reason for its invention in 1952.<sup>40</sup> The fact that this limit was the subject of examinations, despite the model's principal lack of physical realisation, reveals interesting perceptions of models. Consequently this will be discussed in the next section. After having introduced equation 11.2 Stanley implicitly subscribed to Fisher's programme with the words that this equation “will allow us to determine the variation of critical properties of both spin dimensionality  $D$  and lattice dimensionality  $d$ , and thereby to consider a variety of physical systems near their critical points.”<sup>41</sup>

What about the realism of these models? Early in the book, Stanley wrote about this class of models, including the infinite dimensional spin model, that they “are thought to be fairly good approximations to the true interparticle interactions in at least a few physical systems.”<sup>42</sup> However, eq. (11.2) involves several assumptions for all  $D$  and  $d$ ,

[...] that are probably not realistic assumptions for most physical systems that we have been discussing above. These assumptions are made largely in order that the mathematical problem of obtaining critical-point predictions from a model Hamiltonian remains one of manageable complexity. (Stanley; 1971, p. 113)

to serve as a practical model for many systems such as a one-component fluid and a binary alloy.”(Stanley; 1971, p. 111).

<sup>38</sup>Stanley (1971), p. 111.

<sup>39</sup>Stanley (1971), p. 112.

<sup>40</sup>For details, see Kac (1964).

<sup>41</sup>Stanley (1971), p. 113.

<sup>42</sup>Stanley (1971), p. 109.



From considerations of the Heisenberg model and moderate generalisations of the Lenz-Ising model, Stanley concluded that three factors do “not significantly affect the critical-point predictions.”<sup>43</sup> These factors, which concerned the properties of the interactions, were (i) the uniformity of the direction of the interaction between nearest-neighbours ii) the range of interaction (what happens if further than nearest neighbours are taken into account?); and iii) the symmetry of the interaction between two spins (what happens if there is an asymmetry, for instance in the  $z$ -component of the interaction?).

In general Stanley shared the view of the realism of the models expressed by Fisher (1965) and discussed in chapter 8. However, he had a slightly more positive view of the theoretical foundation of the classical Heisenberg model than found in previous accounts of the 1960s, including Fisher (1965).<sup>44</sup> On the other hand, this should not hide the fact that Stanley shared Van Vleck’s view (see page 95) of the two quite restrictive assumptions of isotropy of interaction and well-localised spins on which the classical Heisenberg model is based: “Most magnetic materials in nature fail in one or the other of these two stringent assumptions.”<sup>45</sup>

What role did comparison of model results with experiments play for Stanley? One of the advantages of series expansions is that “they afford the possibility of gauging the validity of a microscopic model by comparison with experiment.”<sup>46</sup> However, this gauging did not have profound consequences for the acceptance or dismissal of the models. In fact, I have only found one instance in the monograph where experimental disagreement was used to justify the dismissal of a model. This was the case with a microscopic model behind the van der Waals theory and the dismissal was done with the words: “Unfortunately such a crude model of interparticle interactions predicts values of the critical-point exponents that are independent of the lattice dimensionality and that disagree with almost all experimental measurements.”<sup>47</sup> As this disagreement is used to introduce the Lenz-Ising model, it must be important for Stanley. However, even though he found it worthwhile to discuss whether or not the critical exponents of the models agree with experiments, even for the case of “a rather unphysical model,”<sup>48</sup> viz. the spherical model, this did not have fatal consequences for the model: it could still be used. By far the most important argument for dismissal of models were their theoretical inadequacies. Furthermore, the comparison of the models with experiments was not at all the scope of his investigations. Rather, the models were used to gain insight into issues belonging to Fisher’s programme.

Even though equation (11.2) covers a lot of ground, it is not impossible to come up

<sup>43</sup> Stanley (1971), p. 113.

<sup>44</sup> Stanley wrote that the perception of this model had changed recently:

[...] it is only within recent years that it has been realized that the classical model is an extremely realistic approximation to the quantum-mechanical case for temperatures near  $T_c$  [...] It is now believed that critical point indices are either independent of spin quantum number  $S$  or they depend on  $S$  so weakly that to an extremely good approximation the spin dependence may be neglected. Hence, although the classical Heisenberg model is an unrealistic approximation to the quantum-mechanical case in the low-temperature domain, it is extremely realistic in the neighbourhood of  $T_c$  as regards critical indices. (Stanley; 1971, p. 112)

<sup>45</sup> Stanley (1971), p. 112. Stanley continued with an echo of Fisher’s view: in recent years materials (including EuO and EuS) have been found “which satisfy both assumptions to a fair extent.” (Stanley; 1971, p. 112) Furthermore, antiferromagnetic materials are known to exist which are “probably well described by the Heisenberg interaction,” (Stanley; 1971, p. 112) such as  $\text{RbMnF}_3$ .

<sup>46</sup> Stanley (1971), p. 165.

<sup>47</sup> Stanley (1971), p. 109.

<sup>48</sup> Stanley (1971), p. 17.

with other models *not* comprised by this equation. So, despite the breadth of the treatment of Stanley (1971), it is in fact quite narrow in focus: by and large Stanley discussed four models and their generalisations. This nicely corroborates my assertion that the Lenz-Ising model had come to the fore within critical phenomena. However, Stanley seem to place more interest on the Heisenberg model than did Fisher. So, it seems that the Lenz-Ising model had to share the position as the preferred model with the classical Heisenberg model.

In his attempt to accomplish Fisher's programme, Stanley summarised previous results and concluded that the values of the critical exponents do *not* depend on the three factors regarding the interaction: i) its directional uniformity; ii) its range (as long as it is of short range); iii) its symmetry. Moreover, he repeated the well-known fact that these exponents do depend crucially on the dimensionality of the lattice. On a less general level, Stanley used the Lenz-Ising model to obtain insight into the latter fact. More precisely, he wanted to "clarify the mechanism whereby nearest-neighbour interactions produce a significant effect between spins that are situated a long distance apart, and this is the essence of what gives rise to critical phenomena and phase transitions in the first place."<sup>49</sup> Based on the Lenz-Ising model he argued that the topology of the lattice determines the path by which two spins on the lattice can interact and therefore also the value of the two-spin correlation function, which shows how a spin at one site in the lattice is correlated with a spin at another site. Since critical behaviour was rightly thought to be due to the large degree of interconnectedness between spins large distances apart, this function reflects the critical behaviour of the system. So, crudely speaking Stanley had established the connection between critical behaviour and dimension, at least for the case of the Lenz-Ising model: "we achieve some insight into the fact that cooperative phenomena (and critical phenomena in particular) depend very sensitively on lattice structure and especially upon lattice dimensionality."<sup>50</sup>

Remarkably, Stanley's basis for these facts of dependence on lattice structure and dimensionality was mainly results on the Lenz-Ising model, rather than experimental data. Generally, the conclusions he drew were supposed to elucidate which features are relevant and which are irrelevant for *real* systems' behaviour. However, once again he relied mainly on facts about model systems such as the above, not experimental results on real systems. In this way these systems had become the main object of study, and it were facts about them which were in need of understanding, as the dimension example illustrates. Stanley's conclusions are only relevant to real systems if the degree of confidence in the model is sufficiently high – if it is believed to be too unrealistic it will not tell anything about the behaviour of real systems. Stanley's argument shows that he must have had a considerable degree of confidence in the model. I believe that this fact reveals quite a change in the perception of the Lenz-Ising model: there is no longer a line drawn between the behaviour of the model on the one hand and the behaviour of real systems on the other. The model is now supposed to give insight into real systems. In short, the model universe had become of central importance to understanding real systems. I shall return to this universe shortly.

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<sup>49</sup>Stanley (1971), p. 148.

<sup>50</sup>Stanley (1971), pp. 165-166.

### 11.4.1 Infinite Spin and the Spherical Model

In the above discussion the spherical model and the infinite spin model stand out because they are not supposed to correspond directly to a real physical system. The spherical model, as already noted by Berlin and Kac (1952), is not a very realistic model of ferromagnetism. Stanley agreed and found that “the spherical model was not very satisfying on various physical grounds,”<sup>51</sup> for example because it allows for “exceedingly unusual possibilities”<sup>52</sup> such as only one spin being non-vanishing while the rest have length zero.<sup>53</sup> However, he wrote,

This statement is not intended to deprecate model systems which as yet have no physical system as a counterpart – there is generally much to be learned from a theoretical model when considered in its own right, and frequently the predictions of the theoretical model motivate a successful search for the appropriate physical system. (Stanley; 1971, p. 17)

Stanley argued that the theoretical model does, nevertheless, shed light on real systems, and it is interesting to consider in what sense he found this to be true. Unfortunately, Stanley did not elaborate on what he more precisely thought could be learned from a theoretical model, but it is reasonable to assume that he referred to insights such as the role played by the infinite spin model in the determination of the variation of critical properties with spin dimension, to which we shall now turn.

The background to the examination of this model was the lack of solvable models on lattices of dimensions higher than one. According to Stanley, the first researcher to study this limit, he “was led to investigate whether any simplifications occurred in the limit  $D \rightarrow \infty$ , that might render the system soluble for lattices of dimensionality  $d > 1$ .”<sup>54</sup> He found that the model “of infinite dimensional spins was in fact quite simple to solve – even for a three-dimensional lattice”.<sup>55</sup>

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<sup>51</sup>Stanley (1971), p. 131.

<sup>52</sup>Stanley (1971), p. 131.

<sup>53</sup>Moreover, “as an approximation to the Ising model, it was essentially a single-shot approximation in the sense that there are no intermediate models that link-up the Ising model and the spherical model.” (Stanley; 1971, p. 131). The situation with regard to experiments is not much better and the agreement between the critical exponents of the model and those found in experimental data is as poor as for the two-dimensional Lenz-Ising model. The value of the spherical model was therefore modest: “The principal virtue to this day of the spherical model result is that it represents one of the very few non-trivial examples of a many-particle system that can be solved exactly for three dimensions.” (Stanley; 1971, p. 17).

<sup>54</sup>Stanley (1971), p. 112.

<sup>55</sup>Stanley (1971), p. 113. He continued:

This was particularly exciting, in as much as only one other non-trivial interacting many-body system has yielded to solution for three-dimensional lattices – namely the Berlin-Kac spherical model (or spherical approximation to the Ising model). Surprisingly, it turns out that the expression for the partition function of  $\mathcal{H}^{(D)}$  in the limit  $D \rightarrow \infty$  is in fact *identical* to the spherical model partition function. (Stanley; 1971, p. 113, emphasis in the original)

This meant that the results obtained by Berlin and Kac for the spherical model were directly applicable to the infinite dimensional spin model.

What did Stanley use the infinite spin model for? In his monograph,<sup>56</sup> the infinite spin model was not merely used as an approximation to the Heisenberg model but had its own place in the framework. The model was discussed in the section where Stanley stated the programme of determining the variation of critical properties with both spin dimensionality and lattice dimensionality. The role of the model in this endeavour is illustrated in table 11.1, taken from Stanley (1971). So, even though the model does not correspond to an existing system, it can be used to study what happens with the critical properties in the limit of infinite spins. In 1999, Stanley stated that this model has played an important role “in the development of current understanding in phase transitions and critical phenomena.”<sup>57</sup> Stanley did not explain why this result is so important, neither in this connection nor in his monograph, but his view might be that it helps capture the dependence of critical behaviour on spin even though no system has infinite spin.<sup>58</sup> The infinite limit gives an extra entry in the classification of models and their critical behaviour. Moreover, due to the solubility of the model, its exponents can be determined exactly, in contrast to what is the case with most models. Such a limit can be used to illustrate, for instance, that the critical exponents vary monotonically with spin dimension. If one accepts this monotonicity, the limit of infinite spin gives a bound on the critical exponents of models with realistic spin dimensions. In this respect it is much similar to the situation with respect to lattice dimension. However, one should not forget that much of the interest in the model relied on the fact that its equivalence with the spherical model made it exactly soluble.

In sum, in his textbook Stanley endorsed completely Fisher's programme and it seems natural to conclude that this endorsement must have been widespread. This was part of a greater trend.

Before closing this section on unrealistic models, we should turn to a paper of 1972 on the application of mathematics by Mark Kac. Here, in a discussion of the use of  $d$ -dimensional spins and the spherical model, Kac had some interesting remarks about the pitfalls of such unrealistic models. In order to appreciate his comments, it is necessary to start with a remark of his on what applied mathematics should *not* be:

I cannot resist referring once more to a wartime cartoon depicting two chemists surveying ruefully a little pile of sand amidst complex and impressive-looking apparatus. The caption read: “Nobody really wanted a dehydrated elephant but it is nice to see what can be done”. I am sure that we can all agree that applying mathematics should not result in creation of ‘dehydrated elephants’. (Kac; 1972, p. 17)

Turning to these models, he wrote: “The models with  $d$ -dimensional spins as well as the spherical model have all the earmarks of being ‘dehydrated elephants’, and it may turn out that indeed they are.”<sup>59</sup> However, Kac thought that they are relevant, but this demands

<sup>56</sup>In the paper where he introduced the relationship between the two models, Stanley gave the following reason: various critical properties were known to be monotonic functions of the spin dimension. “Hence the critical properties of the fairly realistic but hopelessly insoluble Heisenberg model (three-dimensional spins) would appear to be bounded on one side by those of the Ising model (one-dimensional spins) and on the other by those of the spherical model (infinite-dimensional spins).” (Stanley; 1968, p. 718)

<sup>57</sup>Stanley (1999), S362.

<sup>58</sup>A few years after the publication of the monograph Heisenberg models with spin dimensions 0 and even  $-2$  were examined. See Balian and Toulouse (1973) for references. They wrote that they considered the latter case in “[a]n attempt to close the ring[...].” (p. 544).

<sup>59</sup>Kac (1972), p. 26.

arguments:

But what gives these models a hold on life – tenuous though this hold may be – is that in spite of admitted lack of realism, they are firmly *rooted* in *reality*, and they were conceived to deal with *real* questions. Without such rooting and without *real* questions to guide us, we may well find ourselves fighting windmills and triumphantly emerging with pyrrhic victories. (Kac; 1972, p. 26, emphasis in the original)

I think that Kac's statements summarises the view of unrealistic models held by Stanley, Fisher and others nicely: they were perceived to be rooted in reality for the study of real questions.

## 11.5 The Lenz-Ising Model Universe

In addition to its role in the accomplishment of Fisher's programme, the Lenz-Ising model to an increasing extent became a universe which could tell something about the real world. We have already seen in section 10.2 that the Yang brothers suggested that the lattice gas model might explain qualitatively the origin of critical behaviour. Moreover, it was argued above that the model systems had become of central importance to Stanley in his pursuit of understanding real systems. The establishment of this universe provided a framework for a systematic examination of questions about the critical behaviour of real systems.

A good example is how the 'untidiness' of real systems is taken into account. Prior to about 1967, critical systems were almost always treated theoretically as infinite and homogeneous even though they are known to be finite and inhomogeneous. In a testimony that the theory of critical phenomena had reached a stage of maturity where it made sense to move on from the 'justification' of the approach to less fundamental problems such as finite size effects, A. E. Ferdinand and Fisher wrote:

In view of the recently gained insights into the critical-point behavior of the bulk thermodynamic properties of ferromagnets, fluids, alloys, etc., [...], it is appropriate to consider in more detail the corresponding interfacial surface (or boundary) properties and the related distortion of a transition resulting from finite sample size. (Fisher and Ferdinand; 1967, p. 169)

In fact, they wrote two years later, "[r]eal physical systems [...] are finite and possess boundaries, surfaces, and interfaces [...] [F]urthermore, real systems are usually inhomogeneous on some scale containing, for example, impurity atoms, random point defects, grain boundaries, dislocations, nets, strains, etc."<sup>60</sup> All these 'imperfections' are likely to affect the thermodynamical behaviour of the systems and, e.g., 'round' or 'smear' the critical point which is sharp in the 'perfect' system, but their precise effects on the thermodynamics were not known. The most precise experimental measurements did in fact reveal both shifts in the locus of the specific heat peaks and a rounding of this peak.

Several researchers studied theoretically the effect of taking such imperfections into account.<sup>61</sup> Here two papers by Ferdinand and Fisher,<sup>62</sup> will be considered more closely. The details will not interest us; only the structure of their reasoning.

<sup>60</sup>Ferdinand and Fisher (1969), p. 832.

<sup>61</sup>The first to study the finite Lenz-Ising model was Onsager. According to Domb (1996), he himself picked up the thread in 1965. Barber (1983) contains a comprehensive discussion of most of the issues involved.

<sup>62</sup>Fisher and Ferdinand (1967) and Ferdinand and Fisher (1969).

Ferdinand and Fisher studied the impact of interfacial, boundary and finite size effects on the shape and position of the specific heat for the two-dimensional Lenz-Ising model. If this model is finite, its specific heat will not display a singularity as does the infinite model, but will have a maximum. Moreover, the temperature at which the specific heat assumes this maximum is shifted relative to the transition temperature of the infinite model. From calculations they were able to obtain qualitative estimates of the effect of finite sizes for the two-dimensional model. The interesting part for the present discussion, however, is their coupling of these estimates to the real system:

The Ising model in its various forms is known to be a good first approximation for studying the critical behavior of many types of systems [...], our restriction to two-dimensional planar Ising lattices is motivated by a desire for an exact and precise mathematical treatment; we hope that a rigorous knowledge of the two-dimensional behavior will serve as a guide to drawing reliable conclusions about more realistic three-dimensional models. (Ferdinand and Fisher; 1969, p. 833)

Moreover, they concluded, “the detailed exact results found for the square Ising lattice do serve as a check on, and a stimulus to, various heuristic, but more general, arguments concerning the distortion of specific-heat anomalies by finite size.”<sup>63</sup> The adoption of the Lenz-Ising universe implied that they could address the question of the finite-size effect. It is hard to see that this question could have been addressed in a more realistic model, at least in an exact and precise mathematical treatment.

There is some strong evidence that this interest in simple models such as the Lenz-Ising model had become a general movement. There was a lot of efforts in the last years of the 1960s and the early 1970s where such models were examined: The Ashkin-Teller model and the Potts model were proposed much before the 1960s and were not really the focus of interest prior to around 1967. However, in the late 1960s and early 1970s these two were extensively studied.<sup>64</sup> Furthermore, new models were introduced: In 1967, E. Lieb proposed (and solved) the so-called six vertex model in some special cases and a few years later, in 1970, the so-called eight-vertex model was invented by B. Sutherland and, independently, by C. Fan and F. Y. Wu.<sup>65</sup> The importance of such simple models to the understanding of phase transitions and critical phenomena is testified by the fact that the very first volume in the seminal series “Phase Transitions and Critical Phenomena”, edited by C. Domb and M. S. Green, deals with these models as well as the Lenz-Ising model. Moreover, these developments led to the discipline called, as reflected in the title of monograph by R. J. Baxter,<sup>66</sup> ‘exactly solved models in statistical mechanics.’

Such models, despite their unrealism and remoteness from real systems, could tell something about the behaviour of real systems. For instance, following a talk by Joseph E. Mayer, Elliott Lieb made a remark on whether a distinction between two types of phase

<sup>63</sup>Ferdinand and Fisher (1969), p. 185.

<sup>64</sup>A run I performed on Science Citation Index in August 2004, gave the following results: There were four papers citing Ashkin and Teller (1943) in the period from 1945 to 1966, three papers in the time 1967 to 1971, and seven in 1972. The total number of papers citing Ashkin and Teller (1943) in the 1970s was 60. When it comes to the Potts model (citing Potts (1952)), the citation pattern is more or less the same. From 1952 to 1966: two papers; from 1967 to 1971: five papers and in 1972: three papers; the total in the 1970s was 139 papers.

<sup>65</sup>See the first volume of ‘Phase Transitions and Critical Phenomena’ of the 1970s, edited by C. Domb and M. S. Green.

<sup>66</sup>Baxter (1982).

transitions (first and second order) is significant. The important part is not the technicalities of the quotation, but the way Lieb argued:

In Professor Mayer's lecture a large distinction was made between first and second order phase transitions. I should like to raise the slightly heretical point of view that for many systems such a distinction may not be very real. One example of a soluble model is the two-dimensional KDP ferroelectric. In zero field it has a true first order phase transition (latent heat) but in non-zero electric field the transition is second order. Despite the technical difference between the two cases, it is very difficult to discern an 'experimental' difference between the curves for internal energy versus temperature without an electric field or with a small electric field. The curves pass continuously into each other. A parallel example of the opposite sort is the two-dimensional F model antiferroelectric which has an infinite order phase transition in zero field and a second order transition in non-zero field. (Lieb; 1971, pp. 14-15)

Here Lieb argued from the fact that it is difficult to discern whether or not a *model* in a weak electric field exhibits a phase transition of one or the other kind to the conclusion that this should apply to *real* systems.

In short, simple models, and especially the Lenz-Ising model, had become of central importance to the understanding of real systems within critical phenomena and phase transitions in the late 1960s-early 1970s.

## 11.6 Summary of the Use of Simple Models

It has been shown above that in the second half of the 1960s and very early 1970s the Lenz-Ising model was put to a more systematic use in the pursuit of insight into critical phenomena than in the first half of the 1960s. The model played an important role in what I have termed Fisher's programme. According to this programme, to understand critical phenomena means to be able to elucidate what features of the Hamiltonian lead to what kinds of critical behaviour. The latter is characterised by critical exponents. In the accomplishment of this programme, the Lenz-Ising model played an important part, because the programme was quite generally construed. This implied that the effect of the dimensionality of the lattice was seen as relevant (and dimensions different from three were studied), and it was relatively easy to study this effect for the Lenz-Ising model. However, also other models were important and particularly the Heisenberg model was widely used as well.

The second use of the model was through the universe it created. This universe was thought to somehow provide insight into the behaviour of real systems, at least qualitatively. The use of the model in this way had its roots in the first part of the decade, but it was being done much more confidently in the second half. The Lenz-Ising model with its balance between simplicity and realism made it ideal for this purpose: on the one hand, the model was tractable; on the other hand it captured the relevant features of real systems. This application of the model thus demanded a certain confidence in it, viz. that it was in fact capable of describing the essentials of the systems in question. The Lenz-Ising model seems to be indispensable for this job.

However, it was not so much the physical aspects of the models that were in focus. It was not a discussion of the extent to which a particular model was capable of representing

a given physical phenomenon, for instance by comparing the value of the exponents with real materials. Instead, the emphasis was on a quite abstract understanding of the overall features and mechanisms responsible for the critical behaviour.

I believe that Fisher's programme and the accomplishment of it diverges from the approach to modelling phase transitions taken by Joseph E. Mayer. In order to make this divergence, which I think is very fundamental, explicit, I will introduce the notion of *modelling approach*. This notion and the divergence of the two approaches is the subject of the next chapter. However, before turning to this *problématique*, I think it is important to touch briefly upon what caused the change in the second half of the 1960s.

## 11.7 The Cause of the Change

In this chapter I have argued that in the 1960s a change occurred in how models were applied and perceived. The case of Michael E. Fisher, who had worked in the field since the 1950s and who expressed the new view most explicitly, illustrates that physicists who had been in the field of critical phenomena a long time changed their views. Consequently, as it was not only newcomers who held a different view, the change cannot be explained as a generation change.

This raises a question: what was the cause of this change? More specifically: What came first, the change in the perception that the Lenz-Ising model is capable of capturing the essential features of critical points, or the new view of what models were supposed to do? I shall argue that it was the new perception of the Lenz-Ising model which change the view and not the other way round.

As described in the last chapter, most physicists ascribe the change in perception of the Lenz-Ising model to the experiment on argon of Voronel' and co-workers published 1962. This view is supported by the fact that the result of this experiment seems to be heralded as important shortly after its announcement, and by numerous references to it in the literature. Furthermore, Fisher first described his programme in his review paper of 1967, whereas his lecture notes at the Summer Institute for Theoretical Physics at University of Colorado, Boulder in 1964, did not contain such a description. In his lecture notes he did expound the view of the importance of caricature models, but without expressing the more general scope of the programme. It seems fair to assume that Fisher had not conceived his programme at the time of the Summer Institute at least not to such an extent that he revealed anything about it. This is further reflected in his concrete use of the model in the lecture notes, which is restricted to specific problems. Therefore, since Fisher was the first to write about the programme, it is most natural to conclude that it came after the realisation that the Lenz-Ising model does capture many features of certain phase transitions. If this conclusion is correct, Fisher's programme must be seen as an attempt to accommodate the unrealistic model, which nevertheless reveals good agreement with experiments.





# 12

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## Modelling Approaches

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The last chapter showed that the Lenz-Ising model acquired an prominent position within the theory of critical phenomena. However, this position was not simply a matter of whether or not scientists accepted that the Lenz-Ising model can contribute to our knowledge about real systems. In fact, it will be argued in this chapter that the use of the Lenz-Ising model represents an approach to modelling in physics which broke fundamentally with the earlier approaches. As a tool for this discussion, I shall define what I call *modelling approach*.<sup>1</sup> The modelling approach using the Lenz-Ising model is then compared with two other approaches, which had been expounded earlier to deal with particular types of critical phenomena. A more precise characterisation of the notion of modelling approach will be given shortly, but the notion is meant to capture the general features of how phenomena are modelled, detached from the particular phenomena in question. So in principle, a sub-community within, say, the solid state physics community could share a modelling approach with a sub-community within nuclear physics. I start by exemplifying what I have in mind with modelling approach by looking at solid state physics in the 1930s, where several different approaches to the modelling of phenomena were present. After presenting the definition of modelling approach, the three modelling approaches to phase transitions and critical phenomena are placed within this framework. Finally, credence will be given to the claim that the modelling approach using the Lenz-Ising model became, if not the only modelling approach to critical phenomena in the 1960s, then the dominant one within this field.

A word on terminology is called for. In order to distinguish between these three modelling approaches, I have chosen to call the one used within critical phenomena in general the Ising approach, because the (Lenz)-Ising model exemplifies this approach due to its simplicity. Furthermore, this model occupies a prominent place, as both the first and the most studied model of this approach. The second approach is called ‘the Mayer approach’ because Joseph E. Mayer was its most prominent and persistent proponent. Furthermore, the basic model is usually called the Mayer theory or model. I have chosen to call the third approach ‘the Temperley approach’ even though many scientists adhered to this approach because H. N. V. Temperley gave an *explicit* exposition of this approach.

### 12.1 What is Modelling Approach?

Before embarking on giving a precise definition of what I mean by modelling approach, it is worthwhile to consider the solid state physics pioneer Roman Smoluchowski’s description of different approaches to solid state physics. This description brings out what I am hinting at with my notion of modelling approach, even though Smoluchowski is

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<sup>1</sup>The term ‘style’ could be used instead of approach.

concerned with theory rather than modelling, but the difference seems not to be of importance in this context. Based on his 45 years of experience with solid state physicists, Smoluchowski thought it was possible to categorise three types of these physicists in the period from 1930 to the middle of the 1960s (he stated that no nationalistic prejudices were implied by his nationality labels):

The German school was pedantic, basic, rigorous and approached a problem from the point of view of an all-embracing Ansatz. Mathematical difficulties were overcome by sheer force.

The French school was above all elegant and pure. The assumptions may not have been realistic, but the solution was obtainable in a logical, clear manner. The aesthetic beauty of the theory sometimes overshadowed a possible lack of agreement with facts. Ideal lattice and perfect symmetry were *de rigueur* [sic].

The English school was and still is like our common law: the theory may not be elegant or rigorously derivable from some general principles, but it is made to work. Intuition is the crux and models are made and abandoned at the drop of a hat depending on how they work out. It is also, perforce, close to applied problems. (Smoluchowski; 1980, p. 100)

The degree to which Smoluchowski's division is correct or not, is not the point here. Rather, what interests me is that it is possible to point out three approaches whose adherents had divergent opinions concerning the purpose of the modelling, the organisation of the components of the theory, and which models were found acceptable and which were not.

Regarding the degree of detail of a modelling approach it should be sufficiently general so that a given modelling approach is shared by a group of physicists, rather than a single one. Furthermore, a physicist is typically committed to one modelling approach throughout his or her life, so it is only in rare cases that (s)he changes approach.

Needless to say, there is always a wish to gain some kind of insight by modelling, but the type of insights can vary greatly. In a lot of cases insight into a particular phenomenon is in focus; in others the test of a fundamental theory, such as quantum mechanics, is the objective. When a particular phenomenon is in focus, the aim can be either to come up with a detailed quantitative prediction or to provide more qualitative understanding. The phenomenon in question can be either quite specific or more general; for instance the Curie point of a particular ferromagnetic material, the Curie point in general or even transition points in general. Of course, these various phenomena call for different types of explanation or understanding. In some cases, quantum mechanics is required, while in others classical mechanics suffices.

It is tempting to define modelling approach as the common traits of a group of models within a field. However, often a division of labour between the various models occurs, and simply to find the common traits would give a slanted picture of the modelling approach. In the field of ferromagnetism in the 1930s, e.g., people used the Heisenberg model, the Stoner model, the Lenz-Ising model, the spin wave model, the Weiss model, etc. Prior to the 1930s it was found that the Weiss model was able to reproduce experimental results, but it was realised that the model was not based on a theoretically acceptable foundation. Therefore, another model in concordance with first-principles was needed, and the Heisenberg model entered the stage of ferromagnetic models. Heisenberg could show, under some (unjustified) assumptions, that his model led to the molecular field of Weiss's

model. On the other hand, the Heisenberg model was too complicated to be examined in other respects, and the Lenz-Ising model, the spin-wave model and Stoner's model were used. Modelling approach should not, therefore, just be the common traits of the use of the individual models, but also the hierarchy of models and the place of the individual model within this hierarchy.

Even though a foundational theory was known in all the cases of interest in this dissertation, it was not possible in any of them to derive a phenomenological theory (in the sense of section 2.1) of the situation from the foundational theory alone; simplifying assumptions were needed. In this situation, models stepped in and played an important part in the endeavours to build phenomenological theories. In some cases a single model was enough, but often several models were required. This means that one should place the use of a particular model in the context of other models. If one discusses the unrealistic spherical model, e.g., without taking the context of its proposal into account, then one gets a wrong impression of the importance of realism of models within the modelling approach, because the model is used despite its well known unrealism because it is a more tractable model of transition points than the Lenz-Ising model.

Not all features should be counted as parts of a modelling approach. For instance, it is not important whether atoms and not molecules are the basic constituents. However, it is important for the modelling approach that the modelling is an attempt at obtaining macroscopic properties from microscopic units. Another thing which is not counted as part of modelling approach is the mathematical techniques employed. So, even though a lot of efforts were put into developing new mathematical techniques to obtain Onsager's solution of the Lenz-Ising model by other means, I don't think these techniques say anything about the approach to modelling. However, it *does* say a lot about this approach that it had as an ideal that models should be examined in an exact and rigorous way and that some researchers were willing to invest a lot of mathematical effort into examining the model. The main point is that what constitutes modelling approach should be general features.

In sum, I propose the following components in a characterisation of a modelling approach:

1. The overall purpose of the modelling: What kind of insight is it hoped that the model or models will provide?
2. The organisation of the components of the theory: The interplay between the various models.
3. The role played by experimental facts: what kind of confrontation of the models' assertions with such facts is done?
4. Some models are acceptable in the approach, others are not. What criteria are used to distinguish the acceptable from the unacceptable ones?

The exact number of components in the characterisation is not the point here; some would probably use more components, while others would need fewer components. What I want to achieve with the pinning down of these points is mainly to make my characterisation of modelling approach transparent, so it is possible to see which features are included and which ones are excluded. Thus, even though I believe that these components do capture the essential differences in approaches to modelling, I will not try to justify this claim rigorously.

The same purpose can be fulfilled in several different ways, for instance depending on what understanding is perceived to be. The role of the second component (about organisation) is exactly to reveal how one model or several models are used to pursue this purpose.

Agreement with experiments can be expected to be quantitative or qualitative (e.g., should the model predict the value of a critical point or only its existence?), and quantitative agreement can be more or less accurate.

Concerning the fourth component, physicists make a lot of choices: Should the models be based on first-principles or are more *ad hoc* models acceptable? What role should mathematical rigour play in the manipulation of the model? Does the agreement with experimental facts have any role in the acceptance of the theory? Of course many more choices are involved as well.

These components can be illustrated by Smoluchowski's division. Since his division is very brief and the point is illustration, I have taken the liberty to extend his description in some of the cases where it does not give enough information. The purposes ranged from giving intuition (the English school) to putting the phenomena into a general framework in the German school. The French school seems to prefer aesthetic quality to insight into the phenomena under consideration. As to the organisation of the theory, the German school derived consequences from a few fundamental principles, so a single model was used to cover all aspects of the phenomena being studied. In contrast, the English school did not, in principle, defer from employing a new model for every new aspect (this seems to be implied by Smoluchowski's account of the 'unfaithfulness' of the schools to models), so the English school was much more messy than the other two. In the English school agreement with experimental facts is of high priority, while this is not as important to the French school. The models considered to be acceptable differed in two respects: on the one hand, the English school differed from the French and German schools as regards the focus on general principles in the latter two. On the other hand, these two schools differed between themselves because the German school accepted only realistic assumptions (this is my interpretation of Smoluchowski's word "basic"), while this was of less importance to the French school. The French school valued transparency in derivation higher than did the German school, with its adherence to brute force. In other words, Smoluchowski's division illustrates the four components I propose to consider and, more importantly, these components cover all the points taken up by Smoluchowski.

In the following I use the concept of modelling approach to characterise three different approaches to critical phenomena. It has not been possible to find explicit statements about all aspects of modelling approaches for all the three approaches. For instance, the representations of different approaches rarely give concrete expressions of which models are acceptable and which are not. The most serious problem, however, was to determine Mayer's organisation which was not explicitly stated, but had to be inferred from what he actually did. For the cases where explicit statements lack, I have attempted to infer proponents' views from other statements.

## 12.2 Mayer's Modelling Approach

While I think it is possible to single out a by and large coherent group of 1960s physicists committed to more or less the same approach to critical phenomena in general, the group focusing on critical points of *liquids* alone was much less coherent. I will focus on one

author, Joseph E. Mayer and his collaborators, and even though I believe that his views were shared among a larger group, I shall not substantiate this claim here. Mayer and associates studied condensation of gases, including the critical points of liquids, but none of the other critical phenomena, e.g. ferromagnetism, that were treated by the group adhering to the Ising approach.

Before discussing Mayer's modelling approach with respect to condensation, it is worthwhile to consider statements on modelling, which he expressed in relation to other areas of physics than condensation.

In his review from 1957 of Temperley (1956), Mayer gave an interesting classification of approaches to phase transitions:

Statistical mechanical treatments of phase change have never as yet met simultaneously all three criteria of being realistic, rigorous, and numerically applicable. Some treatments manage to satisfy two of these requirements: at least one is rigorous, and treats a realistic model, but does not lead to numerically applicable equations; one is rigorous and numerically applicable, but deals with a model divorced from that of any real material; others treat a reasonable realistic model non-rigorously and arrive at approximate numerical results; most of the rather voluminous literature can not even be said to do as well as meeting even a pair of these three desiderata. (Mayer; 1957, p. 456)

The first model referred to by Mayer is probably his own treatment from the 1930s, while it is likely that he refers to the Lenz-Ising model in his description of the second treatment. The third treatment includes the hard-sphere model.

In a letter to Elliot S. Pierce on July 26 1966, Mayer made the following statement in a referee report of a paper by Grinnel, (the essential is not Grinnel but Mayer's general description of what is important):<sup>2</sup>

My real feeling is that this kind of theory gets nowhere. It is neither fish nor fowl, nor good red meat. One can fit empirical equations without theoretical gobbledegoop and this is useful. One can attempt, rigorous or semi-rigorous theory based on realistic models, in which case mathematical difficulties will probably prevent a close approach to the experimental data, but this may be useful in giving insight into the structure of matter. This attempt of Grinnel's appears to me to be an attempt to draw an elephant with twenty-one parameters, and Poincaré claimed he could do it with five.

There are two important points for the present discussion here. The first is that even though the model does not closely resemble the experimental results, it can still provide insight into matter. The second is a version of Occam's razor that one should not use superfluous parameters.

These quotations show that Mayer was preoccupied with the relation between realism, tractability and experiments.

After these general remarks, we turn to Mayer's treatment of condensation. The overall, but distant, purpose of Mayer and collaborators was, in the words of Kahn, to "explain the general qualitative features of behaviour of gases and liquids." The first three papers of 1937 and 1938, which are the ones treated here, were all steps in this direction but

<sup>2</sup>In Joseph Mayer Papers, Mandeville Special Collection, UC San Diego, Box 2, Folder 15.

concentrated on showing that statistical mechanical methods applied to a gas of  $N$  identical molecules lead to an equation of state that predicts a condensed phase (paper one and two) and “some unexpected phenomena at the critical point”<sup>3</sup> (paper three).

The Mayer treatment gave both qualitative insight and numerical predictions. The qualitative insight was of course about condensation: “The phenomenon of condensation is easily explained by means of these equations.”<sup>4</sup> Here explanation means that a phenomenon analogous to condensation appears in the system. Furthermore, Mayer and Harrison (1938) predicted that the temperature  $T_m$  where the surface tension disappears should be distinguished from the true critical temperature. Regarding the numerical predictions, the treatment gave numerical calculations which could be compared with experimental values. The treatment was supposed to embrace both the condensation of vapours and the particular behaviour of the gas at the critical point. However, Mayer wrote: “We cannot expect the equations of this article, then, without further extension, to give us correct values at the critical point.”<sup>5</sup>

So the general treatment was in principle able to describe both condensation in general and the behaviour at the critical point. However, since this treatment was not tractable in full generality Mayer and coauthors successively coarsened the treatment. At first Mayer and Ackermann restricted the treatment to a system for which the classical mechanical approximations are valid. Secondly, Mayer and Harrison made other restrictions, where the important point is that they considered the method as avoiding arbitrary physical assumptions. So they must consider the fundamental treatment to be quite realistic. Thus the modelling approach of Mayer is to a large extent captured by Smoluchowski’s description of the German school with Mayer’s focus on basic assumptions capable of describing the whole condensation process.

Schematically, the route Mayer followed comprised the following steps:

1. Set up a model of the basic constituents based on reasonable assumptions. This model should be general enough to make it capable of describing several physical phenomena.
2. Attempt to derive the physical consequences of the model.
3. If point 2 is feasible, compare the results with experiments.
4. If point 2 is not feasible, simplify the model.
5. Repeat points 2 to 4 until it is possible to compare the results with experiments.

The existence of a theoretical sound, general treatment gave Mayer and collaborators two advantages: Firstly, it provided a background on which further assumptions could be tested. Of course this gave confidence in the models based on the treatment. On the other hand, a modelling approach which is not based on a general treatment gives more freedom to choose the basic assumptions, and in the case of the Lenz-Ising model, even to choose assumptions contradicting the general treatment. This illustrates one difference between the insights given by the Mayer approach and the Ising approach. Secondly, in principle the general treatment allows for a unified treatment of the whole condensation process from the gas phase to condensation, including the critical point. However, in practice it

<sup>3</sup>Mayer and Harrison (1938), p. 87.

<sup>4</sup>Mayer (1937), p. 71.

<sup>5</sup>Mayer (1937), p. 67.

was necessary to make further assumptions to treat the various parts of the process. In contrast, in the Ising approach it was only possible, even in principle, to treat the, say, the Curie point of ferromagnets and not their general properties.

Mayer's treatment was not second to the Ising approach when it comes to the mathematical level. Like the latter it used a method of extensive mathematical brute force, which resulted in complicatedly looking papers full of multiple integrals, Taylor expansions, sub and super scripts, and almost the entire Latin and Greek alphabets are employed to denote symbols.

Everybody agreed that the Mayer model was realistic and reasonable. One of the main proponents of the Ising approach, Michael E. Fisher, remarked about the Mayer model, in 1965, that the Mayer model is "so familiar that the theorist is apt to forget that it is *only a model* of real physical systems."<sup>6</sup> The nature of the fundamental assumptions, for instance the decay of the interaction energy, makes it very likely that some real systems exists for which they are fulfilled.

Mayer and collaborators dealt primarily with one model (even though they simplified it in the 1960s), which constituted the treatment, so there was no additional components in the theory. This model should not only apply to one particular aspect of condensation, say its critical point, but to the whole range of the behaviour from the gas to the liquid phase, including the particular phase transition at the critical point.

It was important for the Mayer approach adherents that their model could be compared to experiments and they did in fact undertake such comparisons. When it was realised that the prediction of a temperature  $T_m$  is not found in real systems, this did not become a problem for the model, because the prediction was based on non-rigorous arguments. Had the arguments been rigorous this would probably have been a serious problem for the model.

Mayer did not explicitly state which models are acceptable and which are not. Since his model represents condensation and is much more realistic than the lattice gas model, his views on the latter model are of great interest. In a paper coauthored with Howard B. Levine and Henry Aroeste, Mayer treated the lattice gas model, but according to the introduction of the paper, their motivation was mainly to use this model as a stepping stone towards a treatment of liquids based on the more realistic cell method.<sup>7</sup> Mayer did not explicitly express the view that the lattice gas model cannot be used.<sup>8</sup> However, from the quotations above I believe it is possible to infer that he found models which are less realistic than his own of little interest. If I am correct that he tacitly referred to the Lenz-Ising model in his review of Temperley's book with the words that it is "rigorous and numerically applicable, but deals with a model divorced from that of any real material", then he did not seem to consider this model highly. More importantly, if he found, say the lattice gas model, of interest why didn't he consider it? Even if Mayer and his coworkers accepted that the lattice gas model could be vaguely interesting, they never discussed more unrealistic models such as the spherical, Gaussian, or Potts models. That is, their limit of acceptable unrealistic models was the lattice gas model in contrast to the Ising approach adherents who used the mentioned unrealistic models extensively.

<sup>6</sup>Fisher (1965), p. 24, emphasis in the original.

<sup>7</sup>Their paper starts with the sentence: "In order to extend a treatment [...] of liquids based on the cell method, it was found desirable to treat the mathematics of a 'lattice gas' with interaction between neighboring lattice sites." (Levine et al.; 1957, p. 201).

<sup>8</sup>This assertion is based on his published papers and his (unpublished) correspondence available at UC San Diego.



Michael E. Fisher has contrasted his own approach to modelling with what he called the traditional one. He wrote: “The traditional approach of theoreticians, going back to the foundations of quantum mechanics, is to run Schrödinger’s equation when confronted by a problem in atomic, molecular or solid state physics! One establishes the Hamiltonian, makes some (hopefully) sensible approximations and then proceeds to attempt to solve for the energy levels, eigenstates and so on.”<sup>9</sup> Does this description capture the essential features of Mayer’s approach? This approach was explicitly classical and one important aspect in Fisher’s description is that the approach starts from first principles, i. e., quantum mechanics, so his description does not cover the Mayer approach on this fundamental point. This means that even though the Mayer approach and Fisher’s description of the traditional approach are similar in their emphasis of a realistic representation, their spirits are different. Fisher’s description might be adequate for solid-state physics in the early 1930s, but to the best of my knowledge, it does not seem to cover the activities in the subsequent decades.

### 12.3 Temperley’s Modelling Approach

In his monograph,<sup>10</sup> H. N. V. Temperley gave an exposition of another modelling approach. For simplicity I have chosen to name it after him, even though several people, also prior to Temperley’s description of 1956, seem to subscribe to it. Since I haven’t previously given a description of Temperley’s exposition, the following discussion will be more thorough than the description of the two other approaches.

It is clear from various statements of Temperley’s that he considered the realistic interactions to be the relevant ones for theories of phase changes. However, “the resources of statistical mechanics are not yet as to enable us to deduce the rigorous consequences of any realistic molecular interaction function.”<sup>11</sup> So, Temperley was driven towards simpler models out of necessity. Under the heading “Attempts at rigorous theories, using simplified models”, he discussed several such models, including Mayer’s model, the Lenz-Ising model, the Weiss and Bragg-Williams theories. Excepting Mayer’s model explicitly, he wrote about this set of models

It is certainly true that no assembly conforming to [these] types [...] actually exists, nevertheless a comparison of the thermodynamic consequences of such extreme assumptions gives one a clearer idea of what are likely to be the consequences of any *actual* interaction. For example, in a ferromagnetic we are now in a position to compare the consequences of assuming that the interaction is of *very long* range with those of assuming that it is of *very short* range.

<sup>9</sup>Fisher (1983), p. 46. In 1967, Fisher expressed a similar view, namely that the main aim of theory “is sometimes held (implicitly or explicitly) to be the calculation of the observable properties of a system from first principles using the full microscopic quantum-mechanical description of the constituent electrons, protons and neutrons.” (Fisher; 1967, p. 619).

<sup>10</sup>Temperley (1956).

<sup>11</sup>Temperley (1956), p. 22, emphasis in the original. Temperley put forth two criteria to assess a new theory of a change of state in this situation:

- (a) Does it give a satisfying physical picture of what is probably happening?
- (b) Is the numerical agreement with the observed facts in keeping with the number of adjustable parameters, or is the theory unduly “forced” in this respect?

(Temperley; 1956, p. 22)

The consequences of these two extreme assumptions are sufficiently alike to enable tentative conclusions to be drawn about the relationship between the thermodynamic properties of an assembly and the form of the interaction function. (Temperley; 1956, p. 3, emphasis in the original)

This means that the value of such simple models is that they do capture the essential features of more realistic models.

Temperley gave a characterisation<sup>12</sup> of the steps usually taken when a physical theory is developed. He seems to think that theories of phase change should in principle abide to the characterisation, but wrote that so far this has not been possible for any of the models. Indeed, he felt compelled to write down his characterisation because so many attempts have been made to compare the Lenz-Ising model with experiments and “so much confusion has emerged, that it seems worth while to set out the following summary of the logical position.”<sup>13</sup> His characterisation is interesting because it sheds light on his view of the organisation of a physical theory. He wrote:

In developing a physical theory we:

- (a) Choose the model.
- (b) Attempt to derive its quantitative consequences.
- (c) Try to estimate the effects of any approximations we have had to make during step (b).
- (d) Compare the results of (b), as modified by (c), with experiment.
- (e) Try to estimate the effects of generalising the model to include any extra effects known to be present.
- (f) See whether such attempts tend to improve or worsen the agreement between theory and experiment.

(Temperley; 1956, p. 117-8)

From this characterisation it seems natural to conclude that in order for a theory to qualify as a satisfactory physical picture of a phenomenon, Temperley requires that the significance of neglecting known effects (point (e) and (f)) has been examined.

As the starting point for such a discussion of various problems (the exact scope is not clear, but they include alloys, adsorption and related problems), Temperley chose the Lenz-Ising model for two reasons: “[...] first because it is a reasonable first approximation to an interaction of any type that falls off rapidly with distance (though various writers have pointed out that it is not a good representation of the actual quantum mechanical consequences of exchange interaction [...]), secondly because it seems hopeless to try to estimate the probable consequences until we know the correct consequences of this one with reasonable certainty.”<sup>14</sup> So, according to Temperley, one should start with a simple model.

The approximations referred to in (c) are for instance successive approximations such as Bethe's method based on the mean field theory. Here focus is on a small domain of sites, within which the atoms interact correctly, but the atoms on the boundary of the domain

<sup>12</sup>The description appears in a chapter on solutions, but Temperley seems to consider it as more general.

<sup>13</sup>Temperley (1956), pp. 117-8.

<sup>14</sup>Temperley (1956), p. 118.

interact with atoms outside through a mean field. The domain of correctly interacting atoms can be enlarged and by a succession of such enlargements improvement can gradually be obtained. For the sake of completeness, it should be noted that the approximations referred to here do *not* include series expansions.

So, what Temperley argues for in step (e) and (f) is an interactive process between model, theory and experiment, where the effect of making the model more complicated by either refining the effects included or by including altogether new effects.<sup>15</sup> It is not clear, however, what is the next step after (f). If the answer to (f) is that such attempts have no effect, does this mean that the phenomenon in question has now been explained and the process will stop? Or does one attempt to extend the treatment to, say, include other phenomena as well?

Temperley's characterisation can be illustrated by the development of the theory of alloys in the 1930s. As described in Part One, the Lenz-Ising model was examined by using the approximations by Bragg and Williams and by Bethe in the 1930s. This corresponds to step (b) in Temperley's characterisation. However, also his steps (e) and (f) were made in the 1930s. This is clear from the exposition of Nix and Shockley (1938), who wrote:

So far in our theory, the atoms have been rather vague entities. They have been assumed to be distinguishable so that we could designate them by letters *A* and *B* and all their physical properties were exemplified by one or more of the three quantities  $s, v$  and  $V_0$ . Now alloys are far too complicated to be adequately described by such a simple system; and as we shall see in Part II, they frequently depart from theoretical predictions made on this basis. In order to draw the theory nearer to reality, more of the characteristic properties of the metals forming the alloy must be included. In the following sections we describe some preliminary steps made in this direction. (Nix and Shockley; 1938, p. 40)

Next, they mentioned two such steps. One was made by T. S. Chang (1937) who obtained an improvement between theory and experiment by introducing next nearest neighbours into the Bethe approximation.<sup>16</sup> So, Chang examined the role of one of the approximations,<sup>17</sup> i.e. Chang performed steps (e) and (f). Furthermore, Nix and Shockley examined the effect of taking lattice vibrations into account. While not *every* other effect was taken into account, this was another example of Temperley's steps (e) and (f).

Temperley termed such effects not previously taken into account "side effects." He took the estimation of their impact very seriously and the impossibility of such an esti-

<sup>15</sup>In the preface to the second edition of his monograph on statistical mechanics of 1936, Fowler subscribed to something vaguely similar:

Developments in the near future seem likely to consist mainly of applications to more and more complicated models, which are designed to account for more and more subtle properties of matter in equilibrium. Some recent examples of such developments are considered in the new Chapter xxi [on cooperative phenomena] of this edition. (Fowler; 1936b, preface)

<sup>16</sup>Nix and Shockley (1938), p. 40.

<sup>17</sup>However, it is not clear cut whether Chang really examined effect of the approximations of the theory, since his approach leads to two adjustable parameters "that can be varied independently in order to alter the predictions of the theory. With the theories of the origin of the ordering energy in their present state, we regard results obtained by the introduction of further parameters more as an indication of possible types of behaviour than as an explanation of experimental findings." (Nix and Shockley; 1938, p. 41). On the other hand, I think one should look at Chang's intension and it corroborate the wish to test the effect of the approximations.

mation implied that the indeterminacy of the validity of the theory. As a case in point, the theory of magnetism can be used. Since it is not possible to estimate the effect of anisotropy and magnetorestriction (the fact that a magnetic material changes its dimensions when magnetised), Temperley inferred the practical impossibility of item (f). From this he drew consequences which are quite surprising: "At present, then, we are not really in a position to 'decide between' the 'Ising' and 'Weiss' types of model by comparing them with experiments and seeing which gives a better representation of the facts."<sup>18</sup>

The goal of Temperley's work was to understand a particular physical phenomenon and for him a *model* which is known to agree with experiments and where approximations and side effects are controlled, will provide a satisfactory physical *theory*. So, he organised his theory around one model, which is examined, and where the impact of approximations and side effects of the model is investigated by comparison with experimental results.

Experiments played an important role as a testing ground, both for approximations and side effects. The impact of making approximations and neglecting side effects was tested against experimental results. This means that agreement with experimental results was valued highly by Temperley, but he advanced the view that good agreement should not be uncritically taken as corroborating the theory. In fact, he thought that special conditions exist in the case of phase transitions where "some of the accepted criteria of a 'good' or 'bad' scientific theory [break] down completely [...]."<sup>19</sup> In the preface, he stated that for phase transitions "[...], it is not always good enough to find a plausible model that can be made to agree numerically with the observed facts."<sup>20</sup> Later he elaborated his point: If we find that a curve obtained from the model (plus approximations and corrections for "side effects") passes through the experimental points, this "is not *quite* the occasion for rejoicing that it is in other branches of physics [...]."<sup>21</sup> He mentioned the example of spontaneous magnetisation where the mean field model gives a curve which fits the experimental data for iron and nickel, but which is at variance with the Lenz-Ising model. If, on the other hand, we find disagreement between the model and experimental data, "it does *not* follow that we are in a position to find out the cause of the trouble as there may be quite a number of possible explanations."<sup>22</sup>

Temperley accepted simple models, such as the Lenz-Ising model, but only within the field of solutions and adsorption. In his chapters on ferromagnetism and antiferromagnetism and on condensation, the Lenz-Ising model or the lattice gas model are far from being the preferred model. Rather, both chapters deal primarily with much more realistic models, such as the Heisenberg model and the Mayer model. The Lenz-Ising model is mentioned sporadically, but mainly to settle specific issues rather than as the backbone of the theory. So, the Lenz-Ising model was too unrealistic to be used in the field of ferromagnetism and condensation, but in field of alloys and adsorption, where it was generally perceived as being more realistic, it could be used. This reveals that to Temperley the starting point of a theory should not be too simple a model, probably because it would then be out of the question to examine the significance of its side effects.

<sup>18</sup>Temperley (1956), p. 119.

<sup>19</sup>Temperley (1956), pp. 120-121.

<sup>20</sup>Temperley (1956), p. vii.

<sup>21</sup>Temperley (1956), p. 121.

<sup>22</sup>Temperley (1956), p. 121.

## 12.4 The Ising Modelling Approach

The Ising modelling approach was most explicitly stated by Michael E. Fisher. A description of his from 1983 summarised the spirit of this approach:

We should be prepared to look even at rather crude models, and, in particular, to study the relations between different models. We may well try to simplify the nature of a model to the point where it represents a ‘mere caricature’ of reality. But notice that when one looks at a good political cartoon one can recognise the various characters even though the artist has portrayed them with but a few strokes. Those well chosen strokes tell one all one really needs to know about the individual, his expression, his intentions and his character. So, accepting Frenkel’s guidance, [...] a good theoretical model of a complex system should be like a good caricature: It should emphasise those features which are most important and should downplay the inessential details. Now the only snag with this advice is that one does not really know which *are* the inessential details until one has understood the *phenomena* under study. Consequently, one should investigate a wide range of models and not stake one’s life (or one’s theoretical insight) on one particular model alone. Nevertheless, one model which, historically, has been of particular importance and which has given us a great deal of confidence in the phenomenological descriptions of critical exponents and scaling presented earlier deserves special attention: this is the so-called Ising model. Even today its study continues to provide us with new insights. (Fisher; 1983, p. 46-7)

It seems possible to single out a group of people committed to the approach to critical phenomena expounded by Fisher. The group wanted primarily to describe and understand the singular behaviour of critical phenomena. One particular important aspect of this was the similarities and differences between various physical systems, such as liquid gases, ferromagnets and binary alloys. They were not interested in being able to predict the detailed behaviour of such systems. Rather, they wanted to understand why these systems have important similarities in common. Therefore, it did not matter that the critical exponents of the models are only in approximate agreement with experimental results. The goal was simply not to predict the value of exponents.

Most aspects of the Ising approach was described in detail in the last chapter and I shall only give a summary here. On the one hand, realistic models are not tractable mathematically, so it is necessary to consider less complicated models, i.e., caricature models. On the other hand, this necessitates another approach to understanding where one should try to elucidate the relation between the overall features of the Hamiltonian and the critical behaviour. In order to accomplish this, a range of models should be examined rather than one single “fundamental model.” Caricature models are able to do this job. The practical reason is that there is a hope that such models can be examined, even exactly. The fundamental reason is that a good caricature model is capable of capturing the essential features of real systems, so a more complicated model is not needed.

The models functioned in both a negative and a positive way. Already at the time of Onsager, the Lenz-Ising model had this function: if an approximation or a phenomenological theory, such as van der Waals, was at odds with the results on the Lenz-Ising model, the approximation or theory was dismissed. In an area where precise experimental result were notoriously difficult to obtain, the precise numerical values of simple models,

both exact and non-exact, functioned as experimental values and could be used to rule out non-rigorous conjectures and assumptions. However, the simple models also had a positive function. For instance, based on such simple models it was gradually realised that real critical systems are insensitive to the precise nature of the interaction between the constituents.

Experimental facts played a special role. Because the models were so simple, if a disagreement with experiments was found this was not an important issue for a model. Rather, it went the other way round: If agreement was found, that was interesting, because the models were so simple that it was likely that they were at variance with experiments. Because of their lack of realism, the simple models were insensitive to disagreements with experimental results. In fact, the two-dimensional Lenz-Ising model was immune to such disagreements because it was two-dimensional and most real systems cannot be represented in less than three dimensions. Still, the model could work in some contexts.

The adherents to the Ising approach accepted caricature models, such as the Lenz-Ising model, and they mainly examined such models, realising that more realistic models were intractable. Furthermore, they did not stop with the Lenz-Ising model but also considered models even more detached from real systems, such as the infinite spin model, the spherical model and the Potts model. The purpose of studying these models was neither that they would say something direct about real systems, nor that they reveal the behaviour of more realistic, but less tractable models, as Temperley argued. Rather they were interesting due to the light they cast on the correspondence between the features of the Hamiltonian and the critical behaviour.

Those adhering to the Ising approach shared the conviction that explanation and understanding should be based on microscopic models with the two aforementioned modelling approaches. However, the perception of understanding in the Ising approach departed from the perceptions in the two earlier approaches. Previously physicists held the view that a phenomena was understood if it was possible to provide a reasonable model which could reproduce its experimental features. The model was reasonable if it was based on first principles or one could argue that its assumptions were not too unrealistic. On the other hand, the advocates of the Ising approach advanced that “running the Schrödinger equation” is not only infeasible, but does not even provide understanding. Rather, understanding should be sought in caricature models, where focus is on a few characteristic features which are blown up at the expense of other features of the system.

## 12.5 Comparison of the Three Modelling Approaches

The proponents of all three approaches wanted to understand the phenomena in question rather than to predict their detailed behaviour, and they agreed that the models should be of a statistical mechanical nature. However, there was a difference concerning the objects under study. The scope of the Ising approach was the range of different systems under the umbrella ‘critical phenomena,’ while Mayer focused on condensation alone and Temperley dealt with a range of phenomena, but treated each individually. However, one should not overemphasise the importance of this difference in scope. Fisher, for instance, did not try to provide one unified framework for a discussion of all or most of the physical systems under the umbrella ‘critical phenomena.’ Of course he did examine the connection between the phenomena, for instance the analogy provided by the lattice gas model and the magnetic Lenz-Ising model, but by and large he considered each system separately. So

the difference is not that great between the three in this respect.<sup>23</sup> Moreover, the main point with the comparison is to reveal the new features of the Ising approach. To this end, the phenomena studied by the approaches are irrelevant.

Those adhering to the Ising approach had radically different attitudes towards what constitutes understanding than those adhering to either the Mayer approach or the Temperley approach. The former adherents operated with understanding on two levels. They advocated the idea that to understand a physical system means to be able to elucidate which features of the Hamiltonian lead to which types of behaviour of the system. On a more concrete level, to understand a particular aspect of a system means to be able to analyse this feature in a simple model. For instance, the Lenz-Ising model can provide an understanding of the strong dependence of critical exponents on spatial dimensions, because an analysis of the correlation function of the Lenz-Ising model does exhibit the strong dependence of this function on dimension. It should be noted that the Lenz-Ising model could be exchanged with other models of a similar degree of realism.

For Mayer and Temperley understanding, on the other hand, is equal to explanation by a sufficiently realistic model. More precisely, to understand a system means to be able to reproduce its qualitative behaviour of it from a reasonably realistic model. I suppose they would say that only quite realistic models provide understanding. Otherwise, why should they deal with the Mayer model rather than with more unrealistic but more tractable models, such as the lattice gas model? However, Temperley and Mayer disagree about the degree of realism that the models should have: Mayer and associates stressed that their method did not involve arbitrary physical assumptions, while Temperley allowed simplifications (though not as drastic as the adherents to the Ising approach) but only if they could subsequently be checked. So, their concepts of understanding has something in common with the concrete understanding in focus in the Ising approach, but there is a fundamental difference in whether simple models are thought to be able of providing such understanding.

The difference between the Ising approach on the one hand and the Mayer and Temperley approaches on the other concerning this point can be illustrated as follows. Adherents to the Ising approach would say: let us be generous and assume that Mayer and coworkers succeed in, say, obtaining Kahn's goal and were able to describe the whole condensation process. However, this would not have brought us much closer to an understanding of the condensation phenomenon because we would still not be able to point out which characteristics of the system were responsible for what features of the condensation process. In other words, the treatment of Mayer simply mimics the system too well. Turning to Temperley and Mayer and coworkers, they would criticise the approach of the Ising adherents, saying that their models are of mathematical interest only and are too far removed from real materials to say anything about reality.

This difference in the notion of understanding caused a split in the methods used and in the organisation of the phenomenological theory. The Ising approach could not rely on merely one model, because they wanted to elucidate the connection between features of the Hamiltonian, and a single model could not furnish this alone. On the other hand, the Mayer and Temperley approaches both only used a single model (if we consider the original model and the simplifications made in the 1960s as one model in the case of Mayer) because this model was supposed to be sufficiently realistic, so that there was no need to exchange it with another more realistic model. This led to a difference in

<sup>23</sup>Moreover, they all insisted on mathematical rigour in the treatments of these models.

	Ising	Mayer	Temperley
Purpose	Understand critical phenomena in general	Understand condensation phenomena	Understand binary alloys
Organisation	Several models	One model, simplifying	One model, estimating side effects
Experiments	Inexact comparison	Exact comparison	Exact comparison
Acceptable models	Mainly caricature	Only realistic	Simpler than Mayer, but not caricature

**Figure 12.1:** A comparison of the three modelling approaches. The cells are filled out with respect to how the approaches thought things *ought* to be.

organisation of the theory: in the Ising approach a lot of models were taken into account, while the Mayer and Temperley approaches restricted attention to one single model each.

While they agreed on the focus on one model, there is a difference in strategy between the Mayer and Temperley approaches. Whereas Mayer started with a realistic model based on reasonable assumptions which he relaxed when confronted with mathematical difficulties, Temperley advanced the opposite strategy, starting with a simple model whose assumptions were checked.

Another difference between the Ising approach on the one hand and the Mayer and Temperley approaches on the other is their relation to experiments. For the first approach, accurate agreement with experiments could not be expected and consequently even slight agreement would be considered a success of the model. For the two other modelling approaches, accurate agreement would definitely be expected, but the mathematical treatment of the models was far from the state where predictions could be achieved in practice. This meant that Temperley's "programme" to some extent fell apart, with its focus on a interactive process between model and experiments. The Mayer model was of course plagued by even greater mathematical problems, and here agreement with qualitative experimental facts, such as the existence of a critical point, would have been received with enthusiasm. However, such agreement was not possible.

As already noted above, there was a great difference in which models were accepted and which were not by the three approaches. While Fisher used the Lenz-Ising model to gain insight into ferromagnetism, Temperley, along with most people of the 1950s, dismissed the model in this area (Mayer was only preoccupied with the condensation of gas, not with ferromagnetism). For the lattice gas model, the situation is the same: Fisher and associates used the model extensively, whereas Mayer and Temperley restricted their attention to it as a means to get insight into more realistic models. Furthermore, even though the latter two may have found it vaguely interesting, they never discussed more



unrealistic models such as the spherical, Gaussian or Potts models. That is, their limit for unrealistic models was the lattice gas model in contrast to the Ising approach adherents who used the unrealistic models extensively. The Ising adherents did not dismiss the models of the others, but simply considered them to be too complicated to be of interest.

These three modelling approaches are mutually exclusive, in that it is not possible to adhere to two of them at the same time (of course, one can use different modelling approach for different areas or at different times).

The aspects of the Ising approach which were new compared to the other two can be summarised in three points. First, it was accepted that a new class of models, i.e., simple models, could provide both negative and positive results. Second, the adherents to this approach employed a new epistemological strategy. Instead of examining models where the distance to the fundamental theory is short, they used caricature models. Furthermore, instead of making a model progressively more realistic or examine the effect of its assumptions, they examined other models. This new strategy was justified on the terms of a new perception of understanding. Thirdly, the previous two points meant that the task of the theorist changed. Now, it became important to find the significant aspects of the models which could be used for a classification. In practice it was found that the symmetry of the interaction, the spatial dimensions and the spin dimension would do the job. In this classification endeavour, also values of the parameters which were not realised physically, such as infinite spin dimension, were examined. From all this grew a new discipline where models were examined with a focus on mathematical tractability rather than physical realism. The discipline was named “exactly solved models in statistical mechanics,” with a title of a monograph by Baxter (1982).

### Remarks about the Three Strategies

Critical phenomena are too complicated to be examined ‘properly.’ Even though the fundamental theory, i.e. quantum mechanics is well-known and it can be applied directly to this type of phenomena, by making a model which can be considered by and large to be derived from the theory, the examination of the model presents too great mathematical problems for it to be feasible. What do you do when confronted with this situation? There are two possible responses if you want to carry on: i) you make some simplifications of the model, which seem reasonable but cannot be justified theoretically, at least not at first. ii) start all over in the model building process and invent a new model, which is not theory-driven, but more tractable mathematically due to its simplicity.

It is interesting to note that the first strategy was followed by Mayer and his collaborators in the 1960s, while the other was followed by the adherents of the Ising approach.

However, each strategy has its drawbacks: In the first case, if there is an agreement between model and reality it is not certain that it can be ascribed to the model and not the simplifications. However, it is often possible to examine the importance of the simplifications, but sometimes it is not. For instance, the validity of the single electron approximation in solid state physics is not easy to examine. Generally speaking, one will have a high degree of confidence in the model because the ‘distance’ to theory is so short. Another drawback with this strategy is that the simplifications required to make the model tractable may be quite drastical, so that this confidence is lost.

The second strategy has the same drawbacks as the first strategy, but they are more acute because there is no theoretical confidence in the model, due to its lack of theoretical basis. And even worse, it is sometimes close to violating the fundamental theory (e.g., the

Lenz-Ising model of ferromagnetism), which is rarely the case with models representing the first strategy. Furthermore, another difference is that the models of the first strategy are supposed to be applicable to a range of phenomenological behaviours. For instance, the Mayer theory should be applicable not only to critical phenomena, but to condensation in general, and to both sides of condensation, i.e., both gases and liquids. In contrast, the models of the Ising approach are applicable to critical phenomena only. Therefore, the confidence in the first type of models is greater because the models are grounded more broadly.

## 12.6 Dominance of the Ising Approach

The fact that the Lenz-Ising model was extensively used in the 1960s is shown on the graph of the references to Ising (1925) and Onsager (1944) in this period. However, I will argue that much more can be said about the dominance of the Lenz-Ising model, Fisher's programme, and the Ising approach.

The Lenz-Ising model acquired an advanced position within the field of critical phenomena. This is reflected for instance in the papers from the NBS conference on Critical Phenomena. The emphasis was on experimental results,<sup>24</sup> but five major theoretical papers were presented. The papers dealt with the following subjects: "Notes, Definitions, and Formulas for Critical Point Singularities" (Fisher), "Critical Properties of Lattice Models" (Domb), "The Nature of the Cooperative Transition" (Buckingham), "Theory of Critical Fluctuations and Singularities" (Fisher), "Critical Scattering of Neutrons by Ferromagnets" (Marshall). From its title alone it is possible to infer that Domb's paper was placed within the Ising approach. Fisher's first paper dealt with general definitions of the critical exponents but contained a section entitled "Relation Between a Lattice Gas Model and an Ising Magnet", which obviously subscribed to the Ising approach. His second contribution reviewed the 'classical' theories of the behaviour of the correlations close to a critical point. However, evaluation of simple models such as the Lenz-Ising and Heisenberg models was considered to be the most important part. It is not so easy to place Buckingham's contribution, but it dealt with something resembling a lattice gas model. In his theory of scattering, Marshall dealt mainly with Heisenberg's model. Nobody discussed Mayer's model. Joseph E. Mayer himself was invited to chair a session of this conference, but he was unable to attend. He might have presented a dissident view on the conference theme, but his solitary voice would not have drastically altered the theoretical bias of the conference.

So if this conference reflects the state of critical phenomena at the time, and I believe it does, the Lenz-Ising model was preferred to Mayer's model in the field 'critical point of liquid-gas transition,' while both the Heisenberg model and the Lenz-Ising model were considered to belong to the field of ferromagnetism. Binary alloys were not the subject of much interest at the conference, but in this field the Lenz-Ising model had been the

<sup>24</sup>Chairman Green said in his proceedings introduction:

It will be noted that the bulk of the papers at the conference were experimental. This does not represent a bias towards empiricism on the part of the conference organisers but rather their feeling that the most appropriate way to further an eventual theoretical understanding phenomena was by a complete and critical presentation of the experimental situation. (Green; 1966, p. x)

dominant model for a long time, and this was probably the case at the conference as well. So, balancing the score board reveals that the Lenz-Ising model in its various guises (lattice gas model, ferromagnet, antiferromagnet etc.) had acquired a dominant position in the areas of alloys and liquid-gas transition, and a position equal to that of the Heisenberg model in the field of ferromagnets and antiferromagnets.

I have previously argued that Fisher's programme became dominant within critical phenomena. However, even if people subscribed to this programme they need not subscribe to the Ising approach of modelling. However, I will argue that this approach became dominant as well.

It is difficult to measure the degree of support of the Ising approach among scientists within the field of critical phenomena compared to the other approaches. Explicit allegiance to a particular modelling approach is a rare event. However, there are some indications that the Ising approach was the dominant modelling approach. Fisher of course subscribed to it in his influential review of critical phenomena of 1967. Stanley (1971) did so too, more or less explicitly. Moreover there is some circumstantial evidence: The first volumes of the seminal periodical *Phase Transitions and Critical Phenomena* focused on the Lenz-Ising model and similar models rather than on Mayer's model. Furthermore, the large number of papers on such simple models in the late 1960s and the 1970s indicates that many scientists found these models, which were crucial to this modelling approach, of great importance. Would they have examined these models to this extent if they couldn't be used within the greater scheme? Perhaps a few of those participating in the examination of such models, but probably not the far majority.

On other hand not all accepted the Ising approach. Joseph E. Mayer stuck to his own approach, even in the 1960s. I have not been able to find clear indications that Mayer militated against the Ising approach. However, he did not seem to share the interest of this approach in the dimensionality issue. In a letter to the editor of *Journal of Chemical Physics*, J. W. Stout on July 8, 1970 Mayer said: "I am getting a little allergic to one and two dimensional models[...]"<sup>25</sup> More important was his remarks in a "Report on Foreign Travel to attend the Conference on Statistical Mechanics, Trondheim, Norway, June 16-20, 1967" to U. S. Atomic Energy Commission (who sponsored Mayer's research), which he gave in June 30, 1967:<sup>26</sup>

Most of the discussion was mathematical in nature, with very little attention paid to the behavior of the real world. One would have the impression that the universe was two dimensional to hear most of the discussion. This observer was reminded of the fact that the Germans built their first reactor during the war as a two dimensional array, because it was easier to compute. It did not work! However, in spite of the somewhat disturbing lack of real counterparts to the models discussed, there has been a real advance in mathematical technique, and some of this is usable in the more complicated three dimensional case[...]

That he did value a good treatment of a specific model, is revealed by a comment in the same report "The rather short talk by Elliott Lieb [on square ice] was one of the best[...]"<sup>27</sup>

<sup>25</sup>In Joseph Mayer Papers, Mandeville Special Collection, UC San Diego, Box 19, Folder 4.

<sup>26</sup>In Joseph Mayer Papers, Mandeville Special Collection, UC San Diego, Box 2, Folder 19.

<sup>27</sup>In Joseph Mayer Papers, Mandeville Special Collection, UC San Diego, Box 2, Folder 19.

Another dissident was George E. Uhlenbeck,<sup>28</sup> who in a paper with the telling title “Some Historical and Critical Remarks about the Theory of Phase Transitions” of 1978, quite explicitly expressed the view that special models were fundamentally unable to provide answers to the fundamental questions in this field. Uhlenbeck stated these questions as follows:

Why do all substances occur in at least three states of aggregation, the solid, liquid and vapour phase? Why is there a critical point for the vapour-liquid transition and apparently *not* for the fluid-solid transition? These (and many similar) questions are clearly of a *general* nature, and they require a *general* explanation. The questions are *qualitative*; one does not want to calculate precisely, say, what the melting point or the critical point of a given substance are. So the precise details of the intermolecular interactions should not matter. What are the general features of the forces which produce these striking phenomena. (Uhlenbeck; 1978, p. 99-100)

The approach to this problem should reflect its general nature and consequently “Special models may be very instructive, but in my opinion they cannot give the real answer.”<sup>29</sup> This meant that Uhlenbeck dismissed what he called modern theories because, as he wrote, they “have concentrated too much on special models for which exact results could be obtained, and they have neglected the general ‘superstatistical’ features.”<sup>30</sup> Given this characterisation and since Uhlenbeck wrote that they are more exact than van der Waals theory, these theories most include the ones based on the Ising approach. Uhlenbeck did thus disagree fundamentally with this modelling approach on whether it was able to solve the fundamental questions of phase transitions. It should be noted that Mayer’s modelling approach was even more focused on the particular interaction and thus even farther away from Uhlenbeck’s “superstatistical features.” Moreover, it is not clear from his brief paper what Uhlenbeck wanted instead of these modern theories.

The existence of such dissidents does not shake the fact that the Ising approach was dominant by the end of the 1960s – in the words of E. G. D. Cohen, Uhlenbeck was “[...] a man caught on the verge of a transition of one age to a new one[.]”<sup>31</sup> and the same applies to Mayer.

The dominance of the Ising approach is reflected in the quite many textbooks on critical phenomena spanning the time from the 1970s to present time. All of these textbooks, at least the ones I have examined, present the subject matter within the tradition of the Ising approach. This applies to the ones by Stanley (1971), Ma (1976), Toulouse and Pfeuty (1977), Amit (1984) and Goldenfeld (1999). In all of them the Lenz-Ising model plays a special role, and they all share the view on caricature models with Fisher (1967). They rarely subscribe to Fisher’s programme explicitly, which is, however, the underlying philosophy of the texts. It is beyond the scope of my thesis to discuss the impact of the advent of the renormalisation group technique in the 1970s on the acceptance of the Ising modelling approach, but it is likely that this technique played an important role. Roughly speaking, this technique justified the universality hypothesis, which in turn justified the use of simple models. Of course, this does not matter for the fact that the modelling

<sup>28</sup>For an interesting account of Uhlenbeck’s views, including some inconsistencies over time, confer Cohen (1989).

<sup>29</sup>Uhlenbeck (1978), p. 100.

<sup>30</sup>Uhlenbeck (1978), p. 106.

<sup>31</sup>Cohen (1989), p. 623.

approach was accepted, but it shows that one should be careful not to extrapolate from the modern acceptance of the modelling approach to the general acceptance of the modelling approach in the time prior to renormalisation group theory. However, I will not go any further into this discussion.

## 12.7 Summary and Outlook

The above discussion of modelling approaches throws the Ising approach into relief. First of all, it reveals that this approach is not the only one possible and that others have been advocated as well. Furthermore, it illustrated that and how this approach broke with others, mainly in terms of which models are acceptable and of the overall organisation of the theory. It further reveals that the use of caricature models is not as natural as a modern observer might think, because they were not accepted by previous authors such as Temperley and Mayer. This led to a change in the organisation of the theory, which was at serious variance with the organisation of the two other modelling approaches. In fact, I believe that the gap between the Ising approach and the two others is so great that it is reasonable to say that the Ising approach ushered in a new era in the study of critical phenomena. With respect to this field, Fisher's description of two eras of what we today call 'condensed matter physics' given on page 2, is corroborated.

So, the Ising modelling approach diverged drastically from the previous approaches to the modelling of phase transitions and it was definitely a new approach in this area of physics. However, it is certainly possible that a similar approach may have appeared previously in other areas of physics. The extent to which its advent reflected a more general trend within solid state physics is the subject of the next part of the dissertation.

# 13

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## Conclusion of Parts I and II

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It is now time to draw conclusions from the development of the Lenz-Ising model laid out in parts I and II.

I have identified five phases in the development of the perception of the Lenz-Ising model and the role it played. In the first phase, Lenz and Ising proposed the model in the early 1920s as a representation of a ferromagnet. They perceived the model as quite realistic, so there was some disappointment with Ising's conclusion that the one-dimensional model does not exhibit ferromagnetism, while his faulty assertion that this applies to the three-dimensional case as well was not accepted by his contemporaries.

The advent of the new quantum mechanics in 1926-1927 marked the next phase in the development of the Lenz-Ising model. This event changed the foundational theory on which the model was based. When the elementary magnets of the model were reinterpreted in terms of the spins of the new theory, they were found to be strongly distorted representations of these constituents. Consequently, physicists' interest in the model waned in the late 1920s and early 1930s.

In the third phase, which started in the 1930s, the interest in the model grew again, but the motivation was now different. The model was seen as relevant to a study of transition points of cooperative phenomena in general, in contrast to the specific phenomenon of ferromagnetism at the time of Lenz and Ising. Moreover, the role the model was intended to play in the 1930s was new. The background to this was that the mathematical intricacies involved in modelling cooperative phenomena were realised in the 1930s. The prospects that the model might be capable of exhibiting a phase transition, yet at the same time be tractable mathematically, made it ideal for a study of these phenomena. Indeed, Onsager proved in 1944 that the two-dimensional model does display a phase transition. However, Onsager's results did not change the view, also held by Onsager himself, that the model is too far removed from real systems to be directly relevant for a study of such systems. Rather, the model was used as a proof by example that statistical mechanics can accommodate phase transitions. Except for generalisations of Onsager's results, the model was, by and large, perceived as physically irrelevant in the 1950s, except as a representation of alloys. However, one group, Domb's group at King's College examined the model extensively by the use of series expansions. They seem to have held another view of the physical relevance of the model, but this was definitely a minority view.

In the early 1960s, the perception of the model changed fundamentally, and a new phase emerged where the model was confronted with experiments. Agreement was found between the model and some critical exponents within the field of gases, while the Heisenberg model was a more empirically adequate model of magnetism. At any rate, the Lenz-Ising model was used to solve specific small scale tasks, mainly to shoot down hypotheses or phenomenological theories.

In the fifth and final phase, in the last half of the 1960s, the model occupied a prominent position within the theory of critical phenomena and here it was put to a systematic

use. The model played an important role in attempts to fulfil Fisher's programme, which sought to determine the correspondence between features of model Hamiltonians and critical behaviour. The changes in the role of the model in this phase will be described shortly.

I shall now argue that the changes which occurred in the perceptions of the model and the roles it was intended to play in these five phases can be understood in terms of the following four factors:

1. The realism of the model;
2. Mathematical problems involved in modelling;
3. Experimental results; and
4. The overall goal of modelling.

The transition from the first phase to the next was obviously caused by the replacement of foundational theory. The effect was that the *realism* of the Lenz-Ising model suddenly changed its status. This led to a waning interest in the model, since physicists valued the agreement of the model with the foundational theory highly. Consequently, the change in realism led to a change in the role of the model: it was no longer seen as a valid representation of ferromagnets.

I have argued, in contrast to claims by Brush (1967), that the increasing interest in the Lenz-Ising model in the 1930s was mainly due to the realisation of the *mathematical difficulties* of more realistic models of transition points of cooperative phenomena. Therefore, the change of the late 1930s and early 1940s in the perception of the relevance of the model was shaped by the wish to circumvent such difficulties. So, even though the view that the model was far from a realistic representation of ferromagnets had in fact been cemented throughout the 1930s, the model might perform the specific task of being a proof by example of the ability of statistical mechanics to display a phase transition.

So far new experimental results played no role in the perception of the model. However, in the 1960s new experimental results appeared. Some of them showed that the classical theories of critical phenomena are invalid, while others, more importantly, showed that the logarithmic singularity of the specific heat of Onsager's solution also occurred in the real world, namely in the condensation of an argon gas. The latter finding was of course a great success for the Lenz-Ising model, as it was the only model which displayed such a singularity. This meant that all of a sudden the model was no longer seen as a toy model but had acquired status as a caricature model capable of giving insight into real systems. What caused this was *experimental results*.

The model was, however, still perceived as a crude description of the phenomena which it was supposed to represent. This meant that a new attitude towards the purpose of modelling had to be formed. This led to an alteration of how modelling is done and of the task of the theorist. In short, a change in the *overall goal of modelling*. This marks the transition from phase four to phase five.

To sum up, I argue that the four factors are able to describe the changes in the perceptions of the model, but none of them can be left out.

Turning to the roles played by the Lenz-Ising model in the last half of the 1960s, I have argued that the whole attitude towards modelling changed within the field of critical phenomena. In order to describe this change, I have introduced the notion of modelling

approach, which attempts to capture the essence of the handling of models in the pursuit of building phenomenological theories of physical phenomena. In my terminology, a modelling approach is composed of four components:

1. The overarching purpose of the modelling: what kind(s) of insight is it hoped that the model(s) will provide?
2. The organisation of the components of the theory: the interplay between the various models.
3. The role played by experimental facts: what kind of confrontation of the models' assertions with such facts is anticipated.
4. Some models are acceptable in the approach, others are not. What criteria are used to distinguish the acceptable from the unacceptable ones?

I have contrasted the approach to critical phenomena of the 1960s where the Lenz-Ising model was extensively used, and which I therefore call the Ising approach, with two previous modelling approaches. I found that the first approach diverges considerably from those of the other two, mainly with respect to issue one and two: the Ising approach advocates a radical perception of what *understanding* is meant to be in physics. According to the Ising approach the physicist should use a range of simple, tractable models, rather than rely primarily on a single model. These simple models of the Ising approach are of such a nature that the predicate 'caricature' model seems reasonable.

The above considerations answer number one, two and four of the five central questions of section 1.1. There is a final central question that pertains to the development of the Lenz-Ising model. This question (number three) concerns why this model toppled the Mayer model. Except for investigations by a few physicists centred around Joseph E. Mayer, the Mayer model was not examined in the 1960s. The problem was not the assumptions of the model, and there was agreement that it does indeed represent gases faithfully. However, the prospects of solving the mathematical difficulties involved in manipulating the model were far from good. Moreover, in a situation where the simpler (both in mathematical and physical terms) lattice gas model was to some extent successful in reproducing experimental results, the choice of the lattice gas model was natural. Finally, one should not exclude the possibility that the change in the view of the overall goal of modelling played a part as well.

## 13.1 Assessment of the Validity of the Conclusions

It may be worthwhile briefly to review the status of the conclusions drawn above.

Many of these conclusions are based on analyses of two aspects of the physicists' view of the Lenz-Ising model: their perception of the model and of the role the model could play in obtaining insight into real physical phenomena. How well-grounded are these analyses? From a methodological point of view the easy part to obtain is the role of the model, because this is equivalent to the actual use of the model in the research literature, i.e. how models are applied to the phenomena in question. This means that a suitable analysis of the research literature of a given time will reveal this aspect. However, in order to understand why a model can change from being perceived as relevant at one time, irrelevant a little later, and then back to relevant, it is necessary to be able to account in



greater detail for the perception of a model. The perception has a latent component which is not revealed directly in the use of the model and therefore has to be derived in another way.

How I derived the perception of the Lenz-Ising model in the 1950s is exemplary to this discussion, in particular because I argued that the model was perceived as irrelevant in this decade, which is probably the most difficult attitude to detect. I built my argument on a combination of contemporary descriptions of the model and its study (Temperley's textbook<sup>1</sup> and Pais (1958) on the Ising disease), the fact that the model was rarely compared to experiments in this decade, and the views expressed in later recollections by C. Domb, F. Dyson, and C. N. Yang. Concerning the latter views, I believe they can be taken at face value: it is hard to see why Dyson and Yang should want to give an unfavourable impression of the model if this was not reflected in the attitude at the time (one might argue that Domb could in principle have an interest in standing out as pioneer, even though there seems to be no grounds at all for such an accusation). I believe that this combination of materials and evidence makes it reasonable to conclude that the model was in general perceived as irrelevant in this decade – even though the *research* papers on the model in this decade for obvious reasons did not express such a view. On a more general note, this case shows that a detailed and well-grounded account of the perception of a model in a particular epoch can in fact be obtained from such a thorough analysis of a combination of different types of material.

In most cases, a central source for conclusions about the perception of the model at a particular time have been the views about the model expressed in the research papers. The typical way to find papers discussing a particular model is to run Science Citation Index for papers citing an important paper that discusses the model in question. One might worry that such papers will primarily have a *positive* attitude towards the model, while scientists with a negative attitude would not publish papers about the model. So, when the view of the model is derived from the research papers only, the result could be biased, and the perception of the model may be described as more positive than it 'really' was. While this point should cause caution, I think that it is neither as serious as stated nor impossible to circumvent. Firstly, there are in fact examples showing that a physicist's dismissal of a particular model does not hold him back from publishing new results about the model. A case in point is Peierls (1936a), who, as we have seen, showed that the two-dimensional Lenz-Ising model is likely to display a phase transition (in fact, ironically this helped bring the model in from the cold), yet in the same paper dismissed the model as physically uninteresting. So, Peierls did in fact express his negative opinion about the model. There are more examples of this kind, but to put the conclusions on a firmer ground, it would be warranted not to rely too heavily on such research papers alone. Consequently, throughout the dissertation, I have combined the original research papers with textbooks, monographs and review papers, as well as with other sources including letters. This seems to secure a balanced description of the attitudes towards a given model, including those of possible dissidents *vis-à-vis* the majority attitude.

Turning to the five phases and the four factors above, what are their status? My introduction of precisely these five phases is primarily a pragmatic choice: They offered a convenient scheme for a discussion of the perceptions of the Lenz-Ising model and the roles it played over time. I don't think one could do with fewer phases. Perhaps a more refined scheme could be introduced, but I believe that the five phases do in fact capture

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<sup>1</sup>Temperley (1956).

the essential changes in the perception and role of the model.

What about the four factors – are these the ‘right’ ones? It is a fact that the advent of quantum mechanics changed the status of realism of the Lenz-Ising model through the replacement of the foundational theory of the model with a new one. Of course this had an enormous impact on the perception of the model. Based on how Pauli and Peierls described the Lenz-Ising model and its lack of realism in research papers, it is clear that at least these two physicists required a model of ferromagnetism to be in accordance with the new quantum mechanics. There seems to be no reason to think that this view was not widespread. From Pauli’s and Peierls’s descriptions it is therefore justified to conclude that the change in the role of model (that it was no longer relevant for the modelling of ferromagnets) was due to the attitude that the model was not realistic enough.

I have argued that in the next phase it was the interest in transition points of cooperative phenomena in general, rather than, as advanced by Brush, the interest in alloys in particular. My argument built on how Kramers and Wannier, and Onsager, justified taking up the Lenz-Ising model. Since I am interested in the view of the physics community at large rather than the views of these three individuals, it is not so important to ‘cleanse’ the latter views from a possible influence of editors or referees of their papers. Therefore, it seems to be warranted to draw conclusions from how these three presented their papers. Whether this reflects their personal opinions are of less relevance here.

In the last phase, I argue that experiments was the main factor in changing the perception of the model. On the basis of contemporary papers and recollections by Yang, I documented that Voronel’ and collaborators’ experimental results were important. Moreover, it follows from the way other experiments are discussed at the time that they did not play the same role. Moreover, I have excluded the significance of other factors proposed previously on the grounds that they were not advanced by physicists at the time in question.

The arguments for my assertion that it was a new attitude towards the overall goal of modelling which really put the Lenz-Ising model on the map as a model of critical phenomena, are much more elaborate than the previous ones. I have argued that a change occurred in the approach to modelling with the advent of the Ising approach. This is based on a combination of statements about the general task of the theorist, the actual use of the model in reviews and textbooks, and an analysis of the model universe created by the model. The conclusion that the Ising approach broke with previous approaches seems to be well-grounded. That a change in the approach to modelling is needed to explain the prominent role of the model within critical phenomena is shown by the fact that the model was used as a representation of ferromagnetism, even though the agreement between the model and experiments was far from good in this field. So, something in addition to empirical adequacy has to be employed to explain that the model came to occupy a prominent position with the theory of critical phenomena in the latter half of the 1960s. The best candidate for such explanation seems to be the change in modelling approach.

In sum, the conclusion that it was these four factors which changed the phases of the Lenz-Ising model seems to be well-grounded.

Turning to the modelling approaches, I believe that this notion does in fact capture the essentials of the development of modelling in the field of critical phenomena. As shown in the chapter on the three modelling approaches (Chapter 12), the notion is in fact capable of capturing characteristic differences between the three approaches. Moreover, I think that the description does reflect how models are *actually* used. My characterisation of

two of the three modelling approaches, the Ising approach and the Mayer approach, is based primarily on my interpretation of the handling of models in actual practice (in the case of Mayer, there is no exposition of his approach to modelling, so one can only rely on his actual practice). The characterisation of Temperley's approach relies more heavily on the exposition given in his textbook. However, since this exposition is backed by an exemplification of his approach found in the practice of the 1930s physicists, I think it is fair to conclude that his approach is reflected in actual practice, and is not only a description of how he wishes the modelling approach to be. So, I think I can say that my conclusions do in fact apply to the actual practice of physicists and are therefore well-grounded.

How much ground is covered by these three modelling approaches? For the Ising approach it is natural to ask whether my characterisation is adequate for the whole of the modern theory of critical phenomena. I believe I have answered this question in section 12.6. There might be other 'dissidents' than those mentioned, but I think it is fair to say that my characterisation does indeed capture the views of a large and important group of physicists. Concerning the degree of coverage of the two other approaches, if they are to be of real interest, there should be a group of adherents to both. I do find that this is indeed the case. The Mayer approach to condensation is so tightly bounded to his model, that it is fair to say that if people plead for his model, they must somehow subscribe to his modelling approach as well. Since many people subscribed to his model, his modelling approach must have been widespread as well. The Temperley approach is, by and large, the one employed by N. F. Mott. It is actually close to Smoluchowski's description of the English school. If Smoluchowski's description is accepted at face value, this gives credence to the claim that Temperley's modelling approach was widespread too. However, if this conclusion was backed up by other specific studies of actual modelling practice it would be more securely grounded. I have not been able to exclude the possibility of the existence of yet a fourth modelling approach, but it seems difficult to conceptualise how it should differ from the other three. However, one should not rule out the possibility. To sum up, the described modelling approaches do in fact seem to capture essential features of the prevalent approaches to modelling and to cover a lot of ground.

Now the first four of the central questions have been answered. The rest of the dissertation is an attempt to answer the fifth and final question.

## **Part III**

# **A Fundamental Change in Condensed Matter Physics?**



# 14

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## The Hypothesis of a Fundamental Change in Condensed Matter Physics

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There are several indications that condensed matter physics<sup>1</sup> witnessed a considerable transformation in the late 1950s and early 1960s. Michael E. Fisher's view of two distinct eras of the discipline has already been mentioned on page 2. Frederick Seitz (b. 1911), whose career in solid state physics (one of the predecessors to condensed matter physics) started in the 1930s, recalled in an interview in 1981 a change in the organisation of the discipline. Seitz remarked, as a response to the point made by the interviewer Lillian Hoddeson, that solid state physics "looks as though it's coming apart" in the mid-to-late-fifties:

Yes, it exploded into many sub-fields, which happens to fields if they are important. People become very specialized, special techniques, special interests. In addition, of course, the whole business of cooperative phenomena took off. (Seitz; 1981, p. 93)

According to Seitz, the "first inklings"<sup>2</sup> were David Pines's work on so-called collective models of plasmas. Seitz's gave the following response to Hoddeson's question on the significance on the entire field of solid state physics: "Well, it gave one a grip on a new approach."<sup>3</sup>

A third actor, who expressed similar views is Philip W. Anderson (b. 1923) (he is probably correct when he describes himself as a major agenda-setter in condensed matter physics since the 1960s<sup>4</sup>). In his textbook on condensed matter physics, he recalled the years around 1947, when he embarked on his thesis work (on pressure broadening of microwave spectra), as a time characterised by "a very real lack of confidence that any given problems was likely to be soluble [...]".<sup>5</sup> There were many successes in the area of solid state physics at that time, but at the same time most physicists were also "baffled"<sup>6</sup> by the features of a range of phenomena, e.g., antiferromagnetism, superconductivity, and superfluidity. Then he turned to the shift:

I think it is fair to say that in the last 25 or 30 years a quiet revolution has taken place in the methodology and in the confidence with which we ap-

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<sup>1</sup>The umbrella term 'condensed matter physics' for what was previously known as solid state physics and the physics of liquids emerged in the early 1960s. Since the epoch studied in this chapter coincide with the advent of this term, it is justified to use it for the field discussed. However, I will denote the field dealing with the solid state prior to the 1960s by the term 'solid state physics.'

<sup>2</sup>Seitz (1981), p. 93.

<sup>3</sup>Seitz (1981), p. 93.

<sup>4</sup>According to his homepage [http://pupgg.princeton.edu/www/jh/research/anderson\\_philip.html](http://pupgg.princeton.edu/www/jh/research/anderson_philip.html) at Princeton.

<sup>5</sup>Anderson (1984a), p. 4.

<sup>6</sup>Anderson (1984a), p. 4.

proach this subject [...]. A revolution has also, we should hope, come in our predictive success, as well. (Anderson; 1984a, p. 4)

“This success”, he continued, “is based upon a much more rigorous habit of thought combined with a much more complete arsenal of ideas and methods than available[...]” in the late 1950s-early 1960s.<sup>7</sup>

In other words, according to these recollections by Fisher, Seitz, and Anderson, a qualitative change occurred within condensed matter physics in the late 1950s to early 1960s. These three physicists neither elaborated further on the *nature* of the change nor did they document their views. In this chapter I examine, albeit only in outline, a hypothesis which I have formed on the basis of these assertions. The hypothesis consists of two claims: first, that models of a more simplified nature than previously was used to say something about real systems within this field of physics. Secondly, that the *epistemology* of models, i.e. the ways in which models are used to gain insight into the physical world, changed.

The present chapter discusses this hypothesis by addressing three issues: Firstly, does the history of the Lenz-Ising model and the roles it was allowed to play conform with the hypothesis? Secondly, was this approach to critical phenomena really new or can similar tendencies be found prior to the 1960s? Thirdly, to what extent was this approach part of a movement within condensed matter physics around the 1960s?

Of course, in principle one ought to examine the two latter questions for all of condensed matter physics, or at least its most important parts, but that is far beyond the scope of this thesis. Therefore, this discussion is not as systematic as would be desirable, but I believe it is important nevertheless because it outlines a general research programme by pointing to some significant issues. I will rely mainly on memoirs of the scientists in question and only occasionally involve the actual tackling of models.

## 14.1 The Hypothesis and the History of the Lenz-Ising Model

I believe that the history of the Lenz-Ising model and the roles it played laid out in the previous chapters supports the hypothesis. I will not repeat the conclusions here, but only briefly touch upon their bearings on the hypothesis. My study shows that for the Lenz-Ising model the 1960s do indeed mark a watershed: prior to the 1960s, the model was found to be irrelevant as a representation of real physical systems; the model could prove the ability of statistical mechanics to accommodate phase transitions, but it was considered to be too far removed from real systems to say anything more specific about them. This situation changed in the 1960s, when the model acquired a prominent position within the theory of critical phenomena. The acceptance of the model altered the perception of simple or caricature models. They were now thought to be able to actually say something interesting about real systems.

In the 1950s it was well known that the Lenz-Ising model exhibits a phase transition, both in two and three dimensions. Yet only very few physicists examined the model as a representation of real gases or ferromagnets (though it was applied to alloys) in this decade. This reveals that the agenda of 1950s physicists was not simply to provide a model for these two areas, which, in the words of Goldenfeld (see page 20), most economically gives the essential features of the systems. For if this was the agenda, why not treat the simple Lenz-Ising model instead of the more complicated Heisenberg model or Mayer

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<sup>7</sup>Anderson (1984a), p. 4.

model, when the former could very well exhibit the same physics? It seems natural to conclude that these physicists would not accept, because of its lack of realism, the Lenz-Ising model as a representation of the physical systems under consideration. This is contrast to the view of Michael E. Fisher and other adherents to the Ising approach with their emphasis on caricature models. In other words, there seems to be two different attitude towards caricature models on each side of the turn of the 1950s.

Moreover, the history of the Lenz-Ising model and the emergence of the Ising approach reveal a change in the epistemology of models in this area, i.e. how models are used to get insight into real systems. Instead of one single model a range of models were employed to understand critical phenomena.

As far as I can see, this account of the history of the Lenz-Ising model reveals that the development of the model does in fact support the hypothesis. However, I anticipate two objections to this conclusion. Both objections concern whether this attitude of the 1960s really was new.

The first objection was raised by an anonymous reviewer of a draft of my paper on the early history of the Lenz-Ising model (reproduced as part one in this thesis). The reviewer asked about the difference between the use of the Lenz-Ising model in the period around Onsager's solution and the use of statistical mechanical models by British physicists in the 19th century. This issue is discussed in the published paper, but it may be worthwhile to clarify it in the present context. The question of the reviewer will be generalised to adress also the use of the Lenz-Ising model in the 1960s.

The historian of physics Stephen G. Brush has expressed views similar to those of the reader, and it is natural to use Brush's writings to elaborate the issue at hand. In one of his papers, Brush noted that the reasonably good description of a number of phase transitions given by the Lenz-Ising model reveals that the details of the phase transitions are unimportant. From this he concluded:

The success of the Ising model vindicates the approach advocated by Waterston and Maxwell. An atomic model should not incorporate all the physical factors that are believed to influence the system; instead it must be kept simple enough to permit accurate mathematical calculation of its properties. (Brush; 1976, p. 564)

Let us focus on John James Waterston (1811-83) here. Brush had earlier characterised his approach with the words:

Unlike most scientists (before and after him) who worked on the kinetic theory of gases, Waterston wanted only a consistent theory based on a simple model whose properties could be worked out mathematically from a few plausible postulates, rather than a comprehensive flexible theory that could explain all the data. (Brush; 1976, p. 556)

In a sense, Brush is right when he says that Waterston's approach was the same as that taken within critical phenomena in the 1960s: both parties concentrated on a simple model based on a few, not unreasonable assumptions, and both aimed at capturing the essential features of the situation. However, Brush continues with a quotation by Waterston which, I believe, questions the similarity of the two approaches on a deeper level: "Whether gases", Waterston said, "do consist of such minute elastic projectiles or not, it seems worthwhile to inquire into the physical attributes of media so constituted, and to



see what analogy they bear to the elegant and symmetrical laws of aeriform bodies.”<sup>8</sup> Waterston could not know whether gases are made of such small balls with the prescribed properties, because at that time there existed no foundational theory which could inform him about the properties and the behaviour of the constituents of gases. This changed with the advent of quantum mechanics which laid a foundation for determining the unknowns of such constituents. Therefore I don’t think that Waterston’s view is necessarily the same as the one held by the advocates of the Lenz-Ising model in the 1960s. The availability of a foundational theory in the latter epoch gave the physicists at that time an epistemological choice: to choose a description of the constituents of the gases which is either close to or far from the foundational theory. Waterston did not have to and, indeed, could not make such a choice. The availability or not of a foundational theory makes a direct comparison of the two approaches impossible because we do not know how Waterston would have used such a theory.

The second objection to the conclusion that the attitude of the 1960s was new goes as follows: how can this attitude be new, when the simple Lenz-Ising model, or a model equivalent to it, was in fact employed in the 1930s? As described in the first part of the thesis, Hans A. Bethe and others used such a model in the theory of alloys in the 1930s. This is the simplest model based on the assumptions that the ordering is due to the interaction between nearest neighbouring atoms and that the atoms are only characterised by the fact that they can be of two types. Since it does give the essential physics, it fulfills Goldenfeld’s definition of a caricature model. Furthermore, why does this use of the Lenz-Ising model not refute the hypothesis? After all, this version of the Lenz-Ising model was used in the three decades prior to the 1960s.

Even though the Lenz-Ising model of an alloy was a caricature model, from the 1930s to beyond the 1960s it was not perceived to be as distorted as the Lenz-Ising model of ferromagnetism. Already in the paper mentioned above, Bethe wrote that binary alloys should be easier to handle than ferromagnetism: “Super-lattices should be similar [to ferromagnets], and one may even hope that it is simpler to treat since it involves no quantum mechanics but only classical statistics.”<sup>9</sup> So, according to Bethe binary alloys need no quantum mechanics. Therefore, the basis of the Lenz-Ising model for alloys must be better than the model as a representative of ferromagnets. Needless to say, this has a rub-off effect on the overall perception of the model as a representation of the two physical systems. Furthermore, in the 1960s Fisher classified the model as a “simple model,” with the Heisenberg model and the Mayer model, but explicitly *not* in the same category as the Lenz-Ising model of ferromagnetism or the lattice gas model, which were called “simpler models.”<sup>10</sup> So, while the model might have been perceived as simple, it was not in the same league as the variant for ferromagnetism or gas. This is further supported by the fact that Fowler in the 1930s could not have considered the model to be totally remote from real materials since he thought it worthwhile to compare results derived from the model with experiments. Therefore, the model was not perceived as distorted a model of alloys as the Lenz-Ising model of ferromagnets or gases. Consequently, the use of this model as a representative of alloys should not be taken as a refutation of the hypothesis.

After having rejected the two objections, I think it is fair to conclude that the history of the Lenz-Ising model does indeed support the hypothesis.

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<sup>8</sup>Brush (1976), p. 564.

<sup>9</sup>Bethe (1935), p. 553.

<sup>10</sup>The picture was the same in Temperley (1956).

## 14.2 Was the Attitude Towards Models in the Ising Approach Really New?

Was the attitude towards models in critical phenomena really new or is it possible to find something similar in early solid state physics? If this attitude was new, how widespread was it? This section is devoted to a discussion of these questions based on the contemporary expositions by two physicists, as well as the recollections of two other physicists. The discussion is necessarily brief and coarse, but I believe it does point out some interesting fronts with respect to these two questions.

Solid state physics emerged as a discipline in the early 1930s,<sup>11</sup> i.e. after the advent of the new quantum mechanics. The latter theory not only laid the foundation for the study of the solid state, but also affected how this field was approached, according to recollections of Peierls in 1980: “In the 1930s we were strongly influenced by the impressive successes of quantum mechanics in clearing up the basic problems of solid state physics, and this was probably responsible for a tendency to concentrate on general points of principle rather than specific cases.”<sup>12</sup> So, in the infancy of solid state physics the emphasis was not on caricature models of distinctive situations. However, as the field developed it turned, in Pauli’s words, into ‘dirty physics,’ where more *ad hoc* assumptions were required.<sup>13</sup> The new state of the field paved the way for the use of caricature models.

If we accept Smoluchowski’s description of different approaches to models outlined on page 168, the English school used caricature models already in the 1930s. Mott, the epitome of the English school, described his program for solid state physics in a review of Frederick Seitz’s monograph ‘Modern Theory of Solids’ (the first textbook on solid state physics) of 1940. Mott argued that the study of solids can only be justified with two ends in view: either for aesthetic reasons, like the pure mathematics of Hardy’s “Apology”,<sup>14</sup> or because it is of value for practical physicists and metallurgists. Mott did not deny any value to the first purpose, but concentrated on the second. “With this end in view,” he continued, “it seems to me more worth while to attempt to correlate observed phenomena and to give a general explanation in terms of atomic physics, than to attempt any sort of quantitative explanation of phenomena so complicated as those that occur in solids.”<sup>15</sup> As an example he mentioned the theory of metals where Wigner and Seitz had provided a very simple explanation of the coherence of metals and had applied the theory quantitatively to sodium.<sup>16</sup> Mott, however, did not think that attempts of making Wigner and Seitz’s treatment more quantitatively correct were worthwhile:

[...] these attempts are usually not very elegant or pleasing, and are too complicated to be helpful or suggestive to the experimental worker. In fact it seems to me that in this field a fact is only worth explaining if it can be explained simply [...]. (Mott; 1941, pp. 623-4)

As an example he used the phase diagrams of metallurgy. If such diagrams can be explained by simple empirical rules, “[...] the explanation is worth while, but if it depends on some long calculation which balances up the energy of one phase against another,

<sup>11</sup>See, e.g., Weart (1992).

<sup>12</sup>Peierls (1980), p. 34.

<sup>13</sup>Peierls (1980), p. 34.

<sup>14</sup>Hardy (1940).

<sup>15</sup>Mott (1941), p. 624.

<sup>16</sup>Mott (1941), p. 623.

it had better remained unexplained.”<sup>17</sup> In his otherwise positive review of Seitz’s book, Mott’s only criticism is related to this point: “[...] it is difficult to separate the important and suggestive theories from the superstructure that has been built on them in the attempt to get quantitative agreement with experiment.”<sup>18</sup> So, Mott’s wish to make the theory of solids valuable to practical oriented scientists made him prefer simple models to more elaborate, quantitative theories.

The Russian physicist Yakov Ilich Frenkel (1894-1952) also argued for the use of caricature models – indeed he seems to be the one who coined the name – but for more epistemological reasons. In 1946, Frenkel wrote:<sup>19</sup>

The more complicated system considered, the more simplified must its theoretical description be. One cannot demand that a theoretical description of a complicated atom, and all the more of a molecule or a crystal, have the same degree of accuracy as the theory of the simplest atom. Incidentally, such a requirement is not only impossible to fulfill, but also essentially useless [...] An exact calculation of the constants characterizing the simplest physical system has essential significance as a test on the correctness of the basic principles of the theory. Once, however, it passes this brilliantly, there is no sense in subjecting it to further tests as applied to more complicated systems. The most ideal theory cannot pass such tests, owing to the practically unsurmountable mathematical difficulties unavoidably encountered in applications to complicated systems. In this case all that is demanded of the theory is a correct interpretation of the general character of the qualities and laws pertaining to such a system. The theoretical physicist is in this respect like a cartoonist, who must depict the original not in all details, like a photographic camera, but simplify and schematize it in a way as to disclose and emphasize the most characteristic features. Photographic accuracy can and should be required only of the description of the *simplest* systems. A good theory of complicated systems should represent only a good ‘caricature’ of these systems, exaggerating the properties that are most difficult, and purposely ignoring all remaining inessential properties. (Frenkel; 1946, pp. 37-38, emphasis in the original).

As an example, Frenkel used the modern theory of metallic bodies, developed in 1925–1929. We see, he wrote, that this theory,<sup>20</sup>

[...] appears sufficiently satisfactory and that a further mathematical treatment of it, which is based on quantum mechanics and quantum statistics, will not *significantly* contribute to its improvement. A good caricature of an arbitrary human being will not be significantly improved by a more accurate and precise presentation of the non-characteristic details of his face or figure. (Frenkel; 1946, p. 38)

Attempts of the 1930s, Frenkel continued, at improvements of the theory of metals have been misguided. One of his examples is the Jensen-Lenz-Gombas theory. In 1932, Hans

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<sup>17</sup>Mott (1941), p. 624.

<sup>18</sup>Mott (1941), p. 624.

<sup>19</sup>In the translation of Tamm (1962), p. 183. I have this source from the writings of Michael E. Fisher, who repeatedly uses it as a view congenial to his own.

<sup>20</sup>My translation, based on a Danish translation by Albena I. Nielsen of parts of Frenkel’s original paper. I am grateful to her for providing that translation.

Jensen and Wilhelm Lenz (yes, it is the one of the Lenz-Ising model!) modified the Fermi-Thomas statistical treatment of the many-electron problem to more general situations than neutral atoms. A few years later, Pál Gombás applied the method to a model of alkali and alkaline earth metals. By adding several correction terms to remedy some errors of the method, Gombás obtained energies which agreed closely with the experimental ones. Frenkel wrote that Gombás's treatment "allows for the acquisition of more precise results and a more perfect likeness between the caricature, or the 'model', and the original", but<sup>21</sup>

[...] they are similar only to a considerably limited extent and at the expense of a disproportionately large effort and mainly by consciously ignoring other features of the original that are related to the collectivisation of the electrons, the type of structure characterising the compounds, and the mechanical properties, which in these complicated theories appear to be as awkward as in the simple theory. (Frenkel; 1946, p. 38)

In addition to the Jensen-Lenz-Gombas theory, Frenkel applied the same criticism to the band theory of Bloch and Peierls and the Wigner-Seitz theory of alkalis. Since the latter two belong to the crown jewels of 1930s solid state physics, it is reasonable to assume that Frenkel's view on the significance of caricature models was not widespread among physicists at the time.

In sum, according to Smoluchowski's recollections one of the three schools of solid state physics, the English one, advocated the use of caricature models. This conclusion is supported by Mott's review, which criticised more complicated treatments of the solid state than his own. Moreover, another leading physicist, Frenkel, also pleaded for the use of caricature models in the 1940s, but with epistemological arguments (similar to Fisher's) rather than the more pragmatic ones employed by Mott.

But were such views of the relevance of caricature models widespread? From Smoluchowski's elaboration of his comments, it is clear that Mott's "very intuitive approach"<sup>22</sup> met a lot of resistance from fellow solid state physicists:

In the 1940s and early 1950s, Mott's almost eclectic point of view was often criticized as being unsound and contrary to the need of a unified all-embracing solid state theory. I remember very well the heated arguments starting with the Metals Conference in Bristol in 1934 and continuing later at nearly all such gatherings including the famous Varenna School in 1952. (Smoluchowski; 1980, p. 100)

At such meetings, Mott would explain his model and compare it to experiments, but, Smoluchowski continued, "To many of us this was not *gründlich* [thorough] enough."<sup>23</sup> However, Mott and co-workers' approach was gradually accepted: "Slowly, slowly the influence of Mott and of his students and the success of their approach became so evident that no one questioned seriously their value."<sup>24</sup> So, in effect, Smoluchowski described a shift from rejection of the approach based on caricature models to partial acceptance of it, which seems to occur after the early 1950s.

The new situation was a state of methodological pluralism about which Smoluchowski concluded: "Fortunately, this multiple approach to solid state physics still exists: those

<sup>21</sup>My translation from Danish.

<sup>22</sup>Smoluchowski (1980), p. 101.

<sup>23</sup>Smoluchowski (1980), p. 100.

<sup>24</sup>Smoluchowski (1980), p. 101.

who want to make a monolithic self-consistent theory and those who prefer to use, more or less, *ad hoc* models and theories and check experimentally their validity.”<sup>25</sup>

So, some physicists used caricature models in solid state physics already in the 1930s, but not everybody subscribed to this approach. In order to assess whether a change in the perception of models occurred in solid state physics in general, and not only within critical phenomena as I have documented, it is necessary to look at the specific use of models in larger parts of solid state physics. The recollections of the actors can show some tendencies, but do not give a detailed picture.

What about the methodology used prior to the 1960s? Were there any similarities with the one advanced in the 1960s? Smoluchowski’s description of his own methodology with its basic, all-embracing *Ansatz* was far from the one of the Ising approach. However, the English school in general and Mott in particular seem to be good candidates for adherents to a methodology close to that of the Ising approach. I shall restrict my attention to the approach of Mott, and even though it is not possible to give this approach the attention it deserves, I believe it is instructive to look at his work on alloys in the 1930s as it illustrates the above question.

According to Smoluchowski, in general Mott’s approach “was based on a sequence of progressively better models [...]”,<sup>26</sup> where the context makes it natural to perceive “better models” as equivalent to more realistic models. This was not the strategy taken by adherents to the Ising approach. Michael E. Fisher, for instance, put forward the view that one should go in the opposite direction and use progressively *simpler* models.

Turning to Mott’s specific treatment of alloys, this conclusion is supported. He examined the validity of the assumptions of Bethe’s theory of the order-disorder transition of alloys in a paper of 1936 entitled “The Energy of the Superlattice in  $\beta$  Brass.” Based on the theory of metals, Mott estimated the energy required to destroy the superlattice. From this estimate, he concluded about Bethe’s assumption that the work done when a copper atom and a zinc atom exchange lattice sites only depends on their nearest neighbours:

For an ionic lattice such as NaCl Bethe’s assumption would not be correct; if a cation and an anion were interchanged a dipole would be formed, and the extra potential due to it would fall off as  $r^{-2}$ . These long-range forces cannot however exist in a conductor; in  $\beta$  brass, if a pair of copper and zinc atoms change places the conduction electrons will rearrange themselves round the dipole so formed in such a way as to screen it. (Mott; 1936, p. 262)

Mott obtained an estimate for the potential in the neighbourhood of a dipole and concluded from its rapid decrease that it is probably correct to assume that only nearest neighbours interact. “On the other hand”, he continued, “it is probably not true that the interaction energy between a copper atom and a zinc atom is independent of the degree of order of their neighbours.”<sup>27</sup> From a few qualitative arguments concerning how this affects the behaviour of the models, Mott concluded that this might be able to explain a discrepancy between theory and experiment. So, Mott seems to follow Temperley’s strategy of employing a simple model, *in casu* the Bethe model, examine the agreement with experimental results, and then estimate the effect of the assumptions of the model.

The results of this brief discussion of the time prior to the 1960s are the following. Not all solid state physicists, Seitz and Smoluchowski are examples, employed caricature

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<sup>25</sup>Smoluchowski (1980), p. 101.

<sup>26</sup>Smoluchowski (1980), pp. 100-1.

<sup>27</sup>Mott (1936), p. 262.

models, but at least some physicists, such as Mott and Frenkel, used or pleaded for the use of caricature models prior to the 1960s. Even though the adherents to the Ising approach were not the first to use such models, they seem to accept more radical caricature models than did the earlier advocates for such models. On the methodological level, the way Mott used these models diverges from the way the models were employed by the 1960s group interested in critical phenomena. So, if we extrapolate from this brief exposition, the Ising approach does indeed represent a new approach in solid state physics. Admittedly, I have relied mainly on physicists' recollections and contemporary general descriptions of the approach, with all the bias inherent in such expositions. I have only looked at one actual instance of dealing with models, Mott's treatment of alloys, which only covers one tiny aspect of Mott's activities. So, it is possible that one would find adherents to the methodology of the Ising approach in other parts of solid state physics at large prior to the 1960s. However, I believe that this discussion does illustrate what needs to be done in order to examine the hypothesis for the time prior to the 1960s.

### 14.3 A General Movement in Condensed Matter Physics?

I don't claim that the approach taken within critical phenomena was the only approach to the modelling of condensed matter phenomena, but in this section I shall argue that it was part of a general movement within this discipline. I will not determine whether this new approach started within the area of critical phenomena or it had its origins elsewhere.

In his address at the Niels Bohr Centennial Symposium in Boston of 1985, Michael E. Fisher expressed clearly the view that the emphasis on simple models are characteristic of modern condensed matter physics, not only critical phenomena:

The basic problem which underlies the subject [condensed matter physics] is to understand the many, varied manifestations of ordinary matter in its condensed states and to elucidate the ways in which the properties of the "units" affect the overall, many variable systems. In that enterprise it has become increasingly clear that an important role is and, indeed, should be played by various special 'models.' It is, nowadays, a triviality that the behavior of dilute gases is universal and in most regards quite independent of the chemical constitution of the molecules or atoms. We no longer regard the universal ideal gas laws as peculiar or mysterious. One should not, therefore, be so surprised that other theoretical models that have been abstracted from complicated physical systems, like the basic Ising and Heisenberg models originally devised for magnetism, take on a life of their own quite regardless of the underlying atomic and molecular physics (for which quantum mechanics does matter). (Fisher; 1988, p. 67)

Needless to say, I have not gone systematically through all the literature of modern condensed matter physics in order to examine whether or not there is general agreement about these views. However, I have come across one condensed matter physicist, Anderson mentioned above, who had reached the same conclusions as Fisher. Anderson had another starting point in condensed matter physics than Fisher, namely in more traditional solid state physics, with a thesis on spectral line broadening of radio frequencies, under the supervision of John H. van Vleck. So, in order to document the breadth of the movement within condensed matter physics, Anderson is an interesting case.

In an interview with the historian Alexei Kojevnikov in 1999, Anderson discussed the common approach within the many-body community in the 1960s. One of the elements of the approach is trying to find “commonality” of phenomena, a notion which he explained as follows:

Try to find the common feature of a lot of different examples. Try to find the model, which will typify, which will tell you the intrinsic nature of the phenomenon without having to go into lots of messy details. The modeling trick is two-fold. This I guess I did understand very early. There are two conflicting goals. One is to simplify and the other is to get a behavior which is really different from the underlying substrate. (Anderson; 1999, p. 48)

As an example he used so-called localization, i.e., mechanisms for pinning down a magnetic moment to a local region. His basic approach was simple: the model “has to be simple enough so I can solve it, but it has to be complicated enough so it shows localization.”<sup>28</sup> In fact, the latter criterium can be hard to satisfy, and “the possibility of over-simplifying is there.”<sup>29</sup>

So, in his characteristic self-aware style, Anderson said that he realised the importance of caricature models “very early,” but it is not clear precisely when this occurred to him (probably not prior to his thesis submission in 1949). However, what is of equal importance is his statement that the significance of such models was not something obvious, but something that had to be realised. Consequently, the view of the importance of such models can not be something every solid state physicists, implicitly or explicitly, agreed upon from 1930s onwards.

More than 20 years earlier Phil Anderson in his Nobel Lecture of 1977 expressed a viewpoint much like Fisher’s about understanding:

Very often such a simplified model throws more light on the real workings of nature than any number of ‘ab initio’ calculations of individual situations, which even where correct often contain so much detail as to conceal rather than reveal reality. It can be a disadvantage rather than an advantage to be able to compute or to measure too accurately, since often what one measures or computes is irrelevant in terms in mechanism. After all, the perfect computation simply reproduces Nature, does not explain her. (Anderson; 1992, p. 382)

Anderson employed a strong ontological thesis to defend this view:

One of my strongest stylistic prejudices in science is that many of the facts Nature confronts us with are so implausible given the simplicities of non-relativistic quantum mechanics and statistical mechanics, that the mere demonstration of a reasonable mechanism leaves no doubt of the correct explanation. This is so especially if it also correctly predicts unexpected facts [...] (Anderson; 1992, p. 382)

So, despite their different starting points, Anderson shared more or less the same views as Fisher, and, more importantly, Anderson thought that these views were not self-evident.

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<sup>28</sup>Anderson (1999), p. 48.

<sup>29</sup>Anderson (1999), p. 48.

Anderson did not work on critical phenomena, but I have also encountered accounts of scientists from this camp expressing similar views. In his modern textbook of 1992 on this subject, Nigel Goldenfeld felt it necessary to distinguish between two diametrically opposing views about the way models are used in statistical mechanics, the traditional one, employed in, e.g, chemical physics, and the modern one using caricature models (see page 20). The second view is the one of the modern theory of critical phenomena, but interestingly for the present discussion, this is not Goldenfeld's example. Instead he took up the Bardeen-Cooper-Schrieffer theory of superconductivity of 1957:

In such a case, it is only important to start with the correct *minimal model*, *i.e.* that model which most economically caricatures the essential physics. The BCS Hamiltonian is the simplest 4 fermion interaction with pairing between time-reversed states that one can write down. In this viewpoint, all of the microscopic physics is subsumed into as *few* parameters, or phenomenological constants, as possible. As we shall see, the existence of such a viewpoint is a consequence of RG [renormalization group] arguments. (Goldenfeld; 1992, p. 33, emphasis in the original)

So, Goldenfeld definitely sees the use of caricature models as part of a larger movement in statistical physics, and this movement did not even start with the modern theory of critical phenomena. However, one should keep in mind that Goldenfeld, born in the year of the BCS-theory, does not express the view of a participant in the early development.

In a selection of 1999 of his own papers, Leo P. Kadanoff, who did participate directly in the early development, noted that the ideas of scaling and universality had spread from the "the little community" involved in second order phase transitions to other areas of physics. More importantly for the present discussion, he noted the impact of the viewpoint of this community on other parts of physics:

Beyond the export of our specific technical methods, we have also exported a point of view, encompassing the way in which one might look at the structure of physics. One image of this structure is that each little world of phenomena is really based upon the physical laws which describe a more fundamental level of reality. This image leads one to a reductionist outlook. Then one would say that the true goal of physics should be to reach deeper and deeper toward the basic laws which describe the fundamental interactions in the world. However, the study of critical phenomena and other topics in condensed matter physics pushes one toward another and complementary image of nature. (Kadanoff; 1999, p. 162)

According to this complementary image the goal of the scientist's studies of a model world is threefold:

First, to expose the fundamental laws in their most general form and to show how they work out in the specific system in hand. Second, to show how this particular level of experience is related to other closely connected parts of reality. And third, to take the ideas generated in the study of this one particular part of the world and apply them to other portions of the world. (Kadanoff; 1999, p. 162)



The modern theory of critical phenomena “is not in any way unique,”<sup>30</sup> but it is exemplary of this image: “[...] it is a particularly successful and beautiful example of the generation of deep ideas about the simplified world of critical fluctuations, about how those are defined by the microscopic behavior, and about how these ideas manifest themselves in macroscopic behavior.”<sup>31</sup> So, according to Kadanoff, a protagonist in several areas of condensed matter physics, critical phenomena participated in the birth of this new image of the goal of the theorist, but it cannot claim a monopoly on this role because other areas helped as well.

To sum up, this cursory look at the literature reveals that several people expressed views similar to Fisher’s that caricature models are used in condensed matter physics in general and not only within critical phenomena. So, it is fair to conclude that the use of caricature models was indeed a movement in time after World War II. Furthermore, the quotations above suggest that such models really came to the fore around the turn of the decade of 1950. On the other hand, the physicists quoted all seem to belong to the same circles of condensed matter physics, and both Fisher and Kadanoff mentioned Anderson as an inspirator for their views. This underlines that it is not possible to conclude anything decisive about the degree to which their views were shared by the group of physicists at large in the field of condensed matter physics.

## 14.4 Conclusion of Part III

I believe I have laid out some indications that the Ising approach to modelling was in fact new in condensed matter physics. Caricature models were used prior to the 1960s, but the models accepted and employed in the Ising approach in the 1960s were of an even more distorted nature than the ones accepted in the previous epoch. When it comes to the methodology, this seems to be new as well. Turning to condensed matter physics more generally, I have mentioned a few physicists within this field who shared Fisher’s views. Anderson’s opinion of what constitutes understanding was quite close to Fisher’s views. He also wrote that the importance of caricature models was not something obvious, but had to be realised. Anderson stated that he himself did this very early, probably after he started on his thesis work. At any rate, a shift seems to have occurred after World War II in the perception of caricature models.

In sum, I think that there are grounds for believing that the hypothesis put forward in the beginning of this chapter is correct. However, I cannot stress strongly enough that these conclusions are based both on too sporadic material and only on remarks and recollections. It should, therefore, be followed up by a thorough analysis of how models were and are used in actual practice. So, I do believe that in this chapter a programme for future research has been sketched.

This concludes the third part of the dissertation. The last of the five central questions of section 1.1 has been answered. Taken together the three parts of the dissertation have treated and discussed all the central questions posed in the introduction.

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<sup>30</sup>Kadanoff (1999), p. 162.

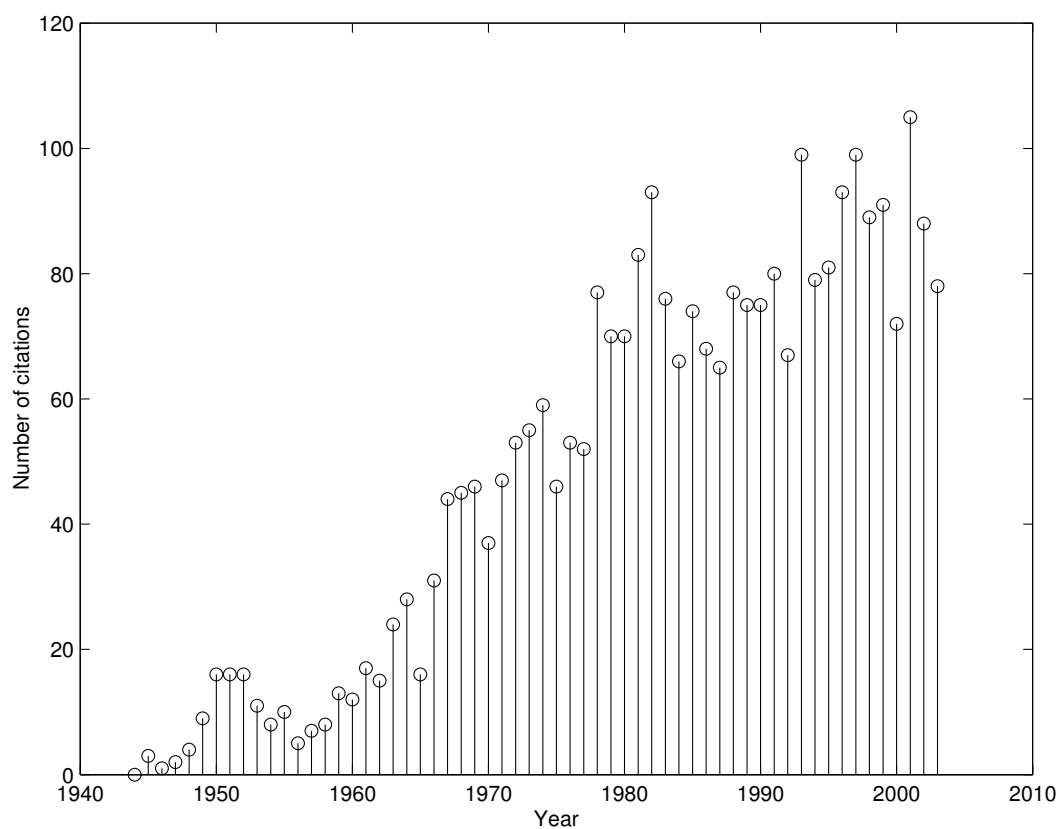
<sup>31</sup>Kadanoff (1999), p. 162.

# Appendices



# A

## Number of References to the Lenz-Ising Model 1945-2003



**Figure A.1:** References to Ising (1925) and/or Onsager (1944).



# B

## Some of the Guises of the Lenz-Ising Model

The mathematical skeleton of the Lenz-Ising model, striped off its physical interpretation, can be defined in the following way: The model ‘lives’ on a lattice and a variable  $s$ , which is allowed to take two values, is placed on each lattice site. A specification of the values of  $s$  for all sites is called a configuration of the model. The Hamiltonian for a configuration is given by

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i. \quad (\text{B.1})$$

We shall use  $\langle ij \rangle$  to denote a sum over nearest-neighbours; the second sum is over all lattice sites.

The variable  $s$  can be given different interpretations depending on the phenomena motivating the model. I shall go through three of the most common ones.

For magnetic systems,  $s$  is a (classical) spin and  $H$  is the strength of the magnetic field imposed on the system. Depending on the value of the exchange energy  $J$ , the model represents various systems. If  $J$  is positive, the spins attempt to align parallel and the mathematical structure is supposed to model *ferromagnetism*. A negative  $J$  favours a antiparallel alignment of spins and the model represents a *antiferromagnet*. If  $J$  is zero, the spins do not interact and only the external field plays a role. This corresponds to a paramagnet.

The Lenz-Ising model can also represent a binary alloy consisting of two species of atoms,  $A$  and  $B$ , living on a lattice and interacting through nearest-neighbours. To this end, the variables are given the following interpretation:

$s_i = 1$  if site  $i$  is occupied by an  $A$  atom,

$s_i = -1$  if site  $i$  is occupied by an  $B$  atom.

The numbers of  $A$  and  $B$  atoms are supposed to be equal and fixed, so  $\sum_i s_i = 0$ . Next, we define  $J_{AA}$ ,  $J_{BB}$ , and  $J_{AB}$ , as the interactions between two  $A$  atoms, two  $B$  atoms and a  $A$  atom and a  $B$  atom, respectively. With these definitions, we may write the Hamiltonian:

$$\mathcal{H} = \frac{1}{4} \sum_{\langle ij \rangle} J_{BB} (1 + s_i)(1 + s_j) + \frac{1}{4} \sum_{\langle ij \rangle} J_{AA} (1 - s_i)(1 - s_j) \quad (\text{B.2})$$

$$+ \frac{1}{4} \sum_{\langle ij \rangle} J_{AB} [(1 + s_i)(1 - s_j) + (1 - s_i)(1 + s_j)]. \quad (\text{B.3})$$

It can be checked by insertion of variables of  $s$  for various pairs of nearest-neighbouring atoms that this Hamiltonian gives the right result. By defining  $J = \frac{1}{4} (J_{AA} + J_{BB} - 2J_{AB})$  and rearranging, the following expression is obtained:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i + C. \quad (\text{B.4})$$

In the lattice gas each site can either be occupied by an atom or be vacant. To this end the following interpretation of  $s$  is used:

$s_i = 1$  if site  $i$  is occupied by an  $A$  atom,

$s_i = 0$  if site  $i$  is vacant.

The Hamiltonian for this system is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - \mu \sum_i s_i, \quad (\text{B.5})$$

where  $J$  is a nearest-neighbour interaction and is taken to be positive, so it favours occupancy of neighbouring sites.  $\mu$  is the chemical potential which controls the number of atoms.

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